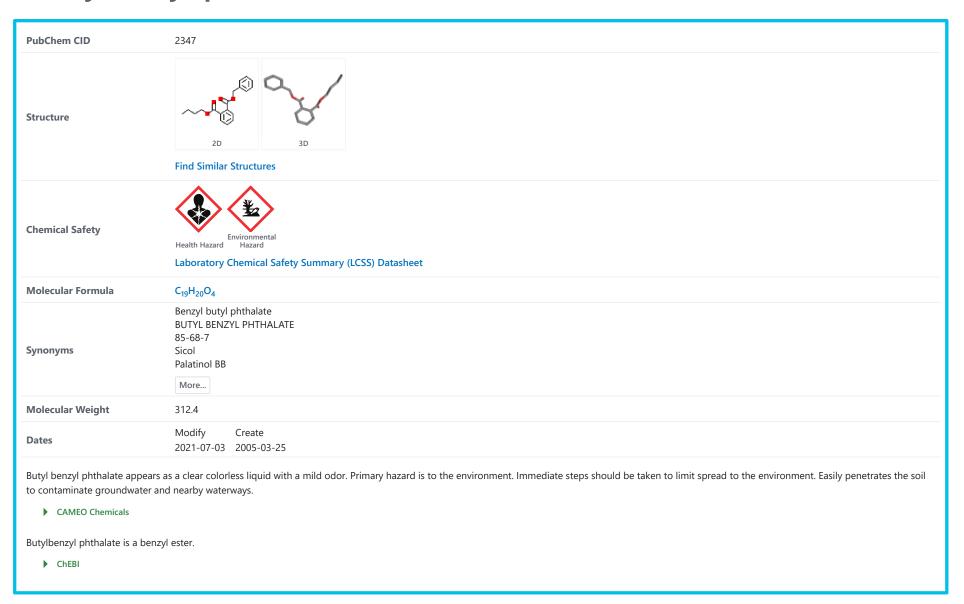


COMPOUND SUMMARY

Benzyl butyl phthalate

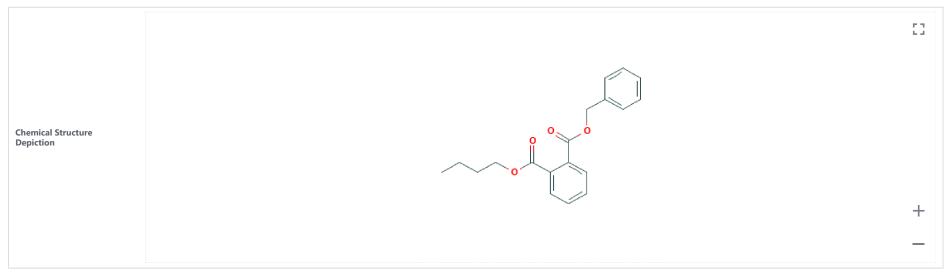


1 Structures

? [2

1.1 2D Structure





PubChem

1.2 3D Conformer

(?) [.

PubChem

2 Names and Identifiers	② 🗵
2.1 Computed Descriptors	② Z
2.1.1 IUPAC Name	② Z
2-O-benzyl 1-O-butyl benzene-1,2-dicarboxylate Computed by LexiChem 2.6.6 (PubChem release 2019.06.18) PubChem	
2.1.2 InChI	② ☑
InChI=1S/C19H20O4/c1-2-3-13-22-18(20)16-11-7-8-12-17(16)19(21)23-14-15-9-5-4-6-10-15/h4-12H,2-3,13-14H2,1H3 Computed by InChI 1.0.5 (PubChem release 2019.06.18) PubChem	
2.1.3 InChl Key	② 🗹
IRIAEXORFWYRCZ-UHFFFAOYSA-N Computed by InChl 1.0.5 (PubChem release 2019.06.18) PubChem	
2.1.4 Canonical SMILES	② Z
CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=C2 Computed by OEChem 2.1.5 (PubChem release 2019.06.18) PubChem	
2.2 Molecular Formula	② Z
C19H20O4 CAMEO Chemicals; ILO International Chemical Safety Cards (ICSC); PubChem	
2.3 Other Identifiers	② Z
2.3.1 CAS	② 🗹

85-68-7

▶ CAMEO Chemicals; CAS Common Chemistry; ChemIDplus; DTP/NCI; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA); Hazardous Substances Data Bank (HSDB); ILO International Chemical Safety Cards (ICSC)

2.3.2 Deprecated CAS	? [2]
58128-78-2	
▶ ChemIDplus	
	0.53
2.3.3 European Community (EC) Number	◎ ☑
201-622-7	
▶ European Chemicals Agency (ECHA)	
2.3.4 ICSC Number	② ☑
0834	
▶ ILO International Chemical Safety Cards (ICSC)	
2.3.5 NSC Number	② Z
71001	
▶ DTP/NCI	
2.3.6 RTECS Number	② Z
TH9990000	
▶ The National Institute for Occupational Safety and Health (NIOSH)	
2.3.7 UN Number	② Z
3082	
▶ CAMEO Chemicals; ILO International Chemical Safety Cards (ICSC); NJDOH RTK Hazardous Substance List	
	0.53
2.3.8 UNII	② Z
YPC4PJX59M	
▶ FDA/SPL Indexing Data	
2.3.9 DSSTox Substance ID	② Z
DTXSID3020205	

▶ EPA DSSTox

2.3.10 Wikipedia

② Z

Benzyl butyl phthalate

Wikipedia

2.4 Synonyms

? [2

2.4.1 MeSH Entry Terms



BBPHT

benzyl butyl phthalate butyl benzyl phthalate

butylbenzyl phthalate

▶ Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms



Benzyl butyl phthalate	Butylbenzylphthalate	DTXSID3020205	CCRIS 104	4mg6
BUTYL BENZYL PHTHALATE	Phthalic Acid Benzyl Butyl Ester	1,2-Benzenedicarboxylic acid, 1-butyl 2-(phenylmethyl) ester	Benzyl butyl phthalate, analytical standard	Benyl n-butyl ph
85-68-7	Phthalic acid, benzyl butyl ester	CHEBI:34595	Santicizer S 160	SpecPlus_00062
Sicol	NCI-C54375	Phthalic acid benzyl n-butyl ester	HSDB 2107	Spectrum2_0018
Palatinol BB	NSC 71001	NCGC00090780-04	EINECS 201-622-7	Spectrum3_0008
Unimoll BB	UNII-YPC4PJX59M	DSSTox_CID_205	BRN 2062204	Spectrum4_0007
Santicizer 160	Butyl phenylmethyl 1,2-benzenedicarboxylate	DSSTox_RID_75431	Benzyl-butylester kyseliny ftalove [Czech]	Spectrum5_0020
Butylbenzyl phthalate	Benzyl-butylester kyseliny ftalove	DSSTox_GSID_20205	AI3-14777	WLN: QVR BVO1
n-Butyl benzyl phthalate	MFCD00009440	Benzyl butylphthalate	benzylbutylphthalate	Phthalic acid bei
Sicol 160	YPC4PJX59M	Caswell No. 125G	benzyl-butyl-phthalate	ACMC-209q7a
Benzyl n-butyl phthalate	2-O-benzyl 1-O-butyl benzene-1,2-dicarboxylate	phenylmethyl 2-(butoxycarbonyl)benzoate	Benzyl butyl phthalated	EC 201-622-7
1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester	Benzyl Butyl Benzene-1,2-Dicarboxylate	CAS-85-68-7	Spectrum_001977	O2-benzyl O1-bı
4				>

PubChem

3 Chemical and Physical Properties

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3.1 Computed Properties

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Property Name	Property Value	Reference
Molecular Weight	312.4	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3	4.9	Computed by XLogP3 3.0 (PubChem release 2019.06.18)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	4	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Rotatable Bond Count	9	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	312.13615911	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	312.13615911	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	52.6 Ų	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	23	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	374	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2019.01.04)

PubChem

3.2 Experimental Properties



3.2.1 Physical Description



Butyl benzyl phthalate appears as a clear colorless liquid with a mild odor. Primary hazard is to the environment. Immediate steps should be taken to limit spread to the environment. Easily penetrates the soil to contaminate groundwater and nearby waterways.

▶ CAMEO Chemicals

Liquid; WetSolid, Liquid

▶ EPA Chemicals under the TSCA

COLOURLESS OILY LIQUID.

▶ ILO International Chemical Safety Cards (ICSC)

3.2.2 Color/Form Clear, oil liquid Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 196 ▶ Hazardous Substances Data Bank (HSDB) ? [7] 3.2.3 Odor Slight odor Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 196 ▶ Hazardous Substances Data Bank (HSDB) ? Z 3.2.4 Taste Bitter David RM et al; Esters of Mono-, Di-, and Tricarboxylic Acids. Patty's Toxicology. 6th ed. (1999-2015). New York, NY: John Wiley & Sons, Inc. On-line Posting Date: 17 Aug 2012 ▶ Hazardous Substances Data Bank (HSDB) 3.2.5 Boiling Point 698 °F at 760 mm Hg (NTP, 1992) National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina. ▶ CAMEO Chemicals 370.0 °C ▶ EPA DSSTox 370 °C Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-44 ▶ Hazardous Substances Data Bank (HSDB); ILO International Chemical Safety Cards (ICSC) 3.2.6 Melting Point less than -31 °F (NTP, 1992) National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina. **▶** CAMEO Chemicals

-35 °C

David RM et al; Esters of Mono-, Di-, and Tricarboxylic Acids. Patty's Toxicology. 6th ed. (1999-2015). New York, NY: John Wiley & Sons, Inc. On-line Posting Date: 17 Aug 2012

▶ Hazardous Substances Data Bank (HSDB); ILO International Chemical Safety Cards (ICSC)

3.2.7 Flash Point



390 °F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

390 °F (199 °C) (Closed Cup)

National Fire Protection Association; Fire Protection Guide to Hazardous Materials. 14TH Edition, Quincy, MA 2010, p. 325-18

▶ Hazardous Substances Data Bank (HSDB)

198 °C

▶ ILO International Chemical Safety Cards (ICSC)

3.2.8 Solubility





less than 0.1 mg/mL at 72.5° F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

8.61e-06 M

HOWARD,PH ET AL. (1985)

▶ EPA DSSTox

In water, 2.69 mg/L at 25 °C

Howard PH et al; Environ Tox Chem 4: 653-61 (1985)

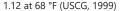
▶ Hazardous Substances Data Bank (HSDB)

Solubility in water, mg/l: 0.71 (very poor)

▶ ILO International Chemical Safety Cards (ICSC)

3.2.9 Density





U.S. Coast Guard. 1999. Chemical Hazard Response Information System (CHRIS) - Hazardous Chemical Data. Commandant Instruction 16465.12C. Washington, D.C.: U.S. Government Printing Office.

CAMEO Chemicals

1.119 g/cu cm at 25 °C

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-44

Relative density (water = 1): 1.1

▶ ILO International Chemical Safety Cards (ICSC)

3.2.10 Vapor Density



10.8 (NTP, 1992) (Relative to Air)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

▶ CAMEO Chemicals

10.8 (Air = 1)

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 12th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2012., p. 501

▶ Hazardous Substances Data Bank (HSDB)

Relative vapor density (air = 1): 10.8

▶ ILO International Chemical Safety Cards (ICSC)

3.2.11 Vapor Pressure





8.6e-06 mm Hg at 68 °F; 1.9 mm Hg at 392° F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

8.25e-06 mmHg

▶ EPA DSSTox

VP: 8.6X10-6 mm Hg at 20 °C

Petrasek AC et al; J Water Pollut Control Fed 55: 1286-96 (1983)

▶ Hazardous Substances Data Bank (HSDB)

8.25X10-6 mm Hg at 25 °C

Howard PH et al; Environ Tox Chem 4: 653-61 (1985)

▶ Hazardous Substances Data Bank (HSDB)

Vapor pressure at 20 °C: negligible

▶ ILO International Chemical Safety Cards (ICSC)

3.2.12 LogP



4.73 (LogP)

ELLINGTON,JT & FLOYD,TL (1996)

▶ EPA DSSTox

log Kow = 4.73

Ellington JJ, Floyd TL; Octanol/water partition coefficients for eight phthalate esters. EPA/600/S-96/006, Sept. 1996; Athens, GA: USEPA, National Exposure Research Lab (1996)

▶ Hazardous Substances Data Bank (HSDB)

4.77

▶ ILO International Chemical Safety Cards (ICSC)

3.2.13 Henrys Law Constant

② Z

Henry's Law constant = 1.26X10-6 atm-cu m/mol at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of Mar 24, 2015: https://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

▶ Hazardous Substances Data Bank (HSDB)

3.2.14 Stability/Shelf Life



Stable under recommended storage conditions.

Sigma-Aldrich; Material Safety Data Sheet for Benzyl butyl phthalate, Product Number: 308501, Version 5.4 (Revision Date 01/02/2015). Available from, as of March 11, 2015: https://www.sigmaaldrich.com/safety-center.html

▶ Hazardous Substances Data Bank (HSDB)

3.2.15 Autoignition Temperature



451 °F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

425 °C

▶ ILO International Chemical Safety Cards (ICSC)

3.2.16 Decomposition

3.2.17 Heat of Combustion



When heated to decomposition, it emits acrid smoke and irritating fumes.

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 401

▶ Hazardous Substances Data Bank (HSDB)



-14,550 BTU/LB= -8,090 CAL/G= -338X10+5 JOULES/KG

U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5.

▶ Hazardous Substances Data Bank (HSDB)

3.2.18 Refractive Index

?

Index of refraction: 1.535-1.540 at 25 °C/D

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: https://monographs.iarc.fr/ENG/Classification/index.php, p. V29: 194 (1982)

▶ Hazardous Substances Data Bank (HSDB)

3.2.19 Kovats Retention Index



Standard non-polar	2327, 2271, 2290.6, 2287, 2287, 2290, 2290, 2327
Semi-standard non-polar	2358.9, 2331.2, 2328.3, 2306.6, 2340.7, 2350, 2320.9, 378.4

NIST Mass Spectrometry Data Center

3.2.20 Other Experimental Properties



Specific gravity: 1.116 at 25 °C/25 °C

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 12th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2012., p. 501

▶ Hazardous Substances Data Bank (HSDB)

Conversion factor: 1 ppm = 12.8 mg/cu m

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: https://monographs.iarc.fr/ENG/Classification/index.php, p. V29: 193 (1982)

- ▶ Hazardous Substances Data Bank (HSDB)
- ... Resistance to migration from polymers, low temperature flexibility ... compatibility with polar polymers and additives over a wide range of compositions. /Phthalate esters/ Kayser, R., D. Sterling, D. Viviani (eds.). Intermedia Priority Pollutant Guidance Documents. Washington, DC: U.S.Environmental Protection Agency, July 1982., p. 1-1
- ▶ Hazardous Substances Data Bank (HSDB)

Maximal acidity: 0.37 meg/100 g

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: https://monographs.iarc.fr/ENG/Classification/index.php, p. V29: 194 (1982)

▶ Hazardous Substances Data Bank (HSDB)

For more Other Experimental Properties (Complete) data for BUTYL BENZYL PHTHALATE (6 total), please visit the HSDB record page.

▶ Hazardous Substances Data Bank (HSDB)

3.3 SpringerMaterials Properties



Boiling point

Heat of sublimation Vapor pressure Viscosity

SpringerMaterials

4 Spectral Information		② Z
4.1 1D NMR Spe	ectra	② Z
4.1.1 1H NMR Spec	tra	② Z
Instrument Name	Varian CFT-20	
Copyright	Copyright © 2009-2020 John Wiley & Sons, Inc. All Rights Reserved.	
Thumbnail		

4.1.2 13C NMR Spectra

② Z

Source of Sample	Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan
Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

Instrument Name	Varian XL-100
Copyright	Copyright © 2002-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	
Inumbhaii	

SpectraBase

4.2 Mass Spectrometry



Instrument Name	VG70
Source of Spectrum	Chemical Concepts, A Wiley Division, Weinheim, Germany
Copyright	Copyright © 2002-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.

Thumbnail

Instrument Name	8230
Source of Spectrum	Chemical Concepts, A Wiley Division, Weinheim, Germany
Copyright	Copyright © 2002-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

SpectraBase

4.2.1 GC-MS

Showing 2 of 10 View More

MoNA ID	JP001747
MS Category	Experimental
MS Type	GC-MS
MS Level	MS1
Instrument	Unknown
Instrument Type	EI-B
Ionization Mode	positive
	149 100
	91 75.3
Top 5 Peaks	206 37.3
	132 22.0
	123 19.3

SPLASH	splash10-052e-4920000000-89027a8d7d37be6301e0
Thumbnail	
Submitter	University of Tokyo Team, Faculty of Engineering, University of Tokyo
Jubilittei	offiversity of tokyo featil, ractarty of Engineering, offiversity of tokyo

MassBank of North America (MoNA)

MoNA ID	JP001748
MS Category	Experimental
MS Type	GC-MS
MS Level	MS1
Instrument	Unknown
Instrument Type	CI-B
Ionization Mode	positive
Top 5 Peaks	91 100 205 97.8 313 92.6 149 76.2 314 43.1
SPLASH	splash10-0btd-6986000000-58f2dee1ae1482e2ac02
-1 1 1	

Thumbnail

Submitter	University of Tokyo Team, Faculty of Engineering, University of Tokyo

MassBank of North America (MoNA)

4.2.2 MS-MS



NIST Number	1186193
Instrument Type	IT/ion trap
Collision Energy	0
Spectrum Type	MS2
Precursor Type	[M+H]+
Precursor m/z	313.1434
Total Peaks	16
m/z Top Peak	205
m/z 2nd Highest	148.9
m/z 3rd Highest	91

Thumbnail

NIST Mass Spectrometry Data Center

4.2.3 LC-MS



Showing 2 of 5 View More

MoNA ID	SM836901
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M+H]+
Precursor m/z	313.1434
Instrument	Q Exactive Plus Orbitrap Thermo Scientific
Instrument Type	LC-ESI-QFT
Ionization	ESI
Ionization Mode	positive
Collision Energy	35 (nominal)
Retention Time	13.193 min
	91.0542 100
	149.0234 39.7
Top 5 Peaks	205.086 3.2
	65.0387 1.2
	181.0495 0.7
SPLASH	splash10-0006-9300000000-595d7be3b0c3da1a203e

Thumbnail

Submitter CASMI Team, UFZ, Eawag

MassBank of North America (MoNA)

MoNA ID	EQ359701		
MS Category	Experimental		
MS Type	LC-MS		
MS Level	MS2		
Precursor Type	[M+H]+		

Active Plus Orbitrap Themo Scientific		
	Precursor m/z	313.1434
contaction Mode ESI contaction Mode positive collision Energy 15 (nominal) cetertion Time 14.2 min ceter May 1232 65 4 149,0232 65 4 cop 5 Peaks 7,06870 1.5 6,0383 0.4 918xH0 -0007-9510000000-56d5471a666581b26651 PLASH splash10-0007-9510000000-56d5471a666581b26651	Instrument	Q Exactive Plus Orbitrap Thermo Scientific
	Instrument Type	LC-ESI-QFT
15 15 15 15 15 15 15 15	Ionization	ESI
letention Time	Ionization Mode	positive
10,942 100 149,0232 65.4 20,0859 16.8 57,0697 0.5 50,383 0.4 PLASH splash10-0007-951000000-56d5471a6b6581b26651 humbhail	Collision Energy	15 (nominal)
149,023 2 65.4 205.0859 16.8 57.0697 0.5 65.0383 0.4 PLASH splash10-0007-951000000-56d5471a6b6581b26651 humbnail	Retention Time	14.2 min
PLASH splash10-0007-9510000000-56d5471a6b6581b26651 humbnail	Top 5 Peaks	149.0232 65.4 205.0859 16.8 57.0697 0.5
humbnail	SPLASH	
ubmitter Eawag Team, Eawag - Swiss Federal Institute of Aquatic Science and Technology	Thumbnail	
	Submitter	Eawag Team, Eawag - Swiss Federal Institute of Aquatic Science and Technology

MassBank of North America (MoNA)

4.3 IR Spectra

4.3.1 FTIR Spectra

Showing 2 of 9 View More

Technique	BETWEEN SALTS
Source of Sample	BASF AG / BASF Corporation
Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

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Technique	NEAT (KBr)
Source of Spectrum	SRL
Source of Sample	Monsanto Company, St. Louis, Missouri
Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

SpectraBase

4.3.2 ATR-IR Spectra

(?)	
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Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DurasampliR II)

2021	Berizyi butyi pintialate 0 19112004 - 1 ubonem
Source of Spectrum	Forensic Spectral Research
Source of Sample	Scientific Polymer Products, Inc.
Catalog Number	P-135
Lot Number	080723001
Copyright	Copyright © 2012-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

Source of Sample

Aldrich

-		
Catalog Number	308501	
Copyright	Copyright © 2018-2020 Sigma-Aldrich Co. LLC Database Compilation Copyright © 2018-2020 John Wiley & Sons, Inc. All Rights Reserved.	
Thumbnail		

4.3.3 Near IR Spectra	
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Technique	NIR Path Length= 0.5/20 Spectrometer= BRUKER IFS 88 Spectrometer= INSTRUMENT PARAMETERS=INST=BRUKER,RSN=10563,REO=2,CNM=HEI,ZFF=2	
Source of Spectrum	Prof. Buback, University of Goettingen, Germany	
Copyright	Copyright © 1989, 1990-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.	
Thumbnail		

Technique	NIR Path Length= 0.5/20 Spectrometer= BRUKER IFS 88 Spectrometer= INSTRUMENT PARAMETERS=INST=BRUKER,RSN=10563,REO=2,CNM=HEI,ZFF=2
Source of Spectrum	Prof. Buback, University of Goettingen, Germany
Copyright	Copyright © 1989, 1990-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
-1 1 1	
Thumbnail	

4.3.4 Vapor Phase IR Spectra



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r ,	11/
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Technique	Vapor Phase
Source of Sample	Aldrich Chemical Company, Inc., Milwaukee, Wisconsin
Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

Technique	Vapor Phase
Source of Spectrum	Sigma-Aldrich Co. LLC.
Source of Sample	Aldrich
Catalog Number	308501
Copyright	Copyright © 2018-2020 Sigma-Aldrich Co. LLC Database Compilation Copyright © 2020-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

4.4 Raman Spectra



Instrument Name	Bruker MultiRAM Stand Alone FT-Raman Spectrometer
Technique	FT-Raman
Source of Spectrum	Bio-Rad Laboratories
Source of Sample	Sigma-Aldrich Company Llc.
Catalog Number	308501
Lot Number	MKBH8959V
Copyright	Copyright © 2014-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

5 Related Records 5.1 Related Compounds with Annotation ② 🖸

PubChem

5.2 Related Compounds

② Z

Same Connectivity	3 Records
Same Parent, Connectivity	6 Records
Same Parent, Exact	4 Records
Mixtures, Components, and Neutralized Forms	15 Records
Similar Compounds	7,952 Records
Similar Conformers	44 Records

PubChem

5.3 Substances

② Z

5.3.1 Related Substances

(?)	Ŀ

All	169 Records	
Same	153 Records	
Mixture	16 Records	

PubChem



PubChem

5.4 Entrez Crosslinks



PubMed	254 Records
Protein Structures	1 Record
Taxonomy	13 Records
Gene	328 Records

PubChem

5.5 Associated Chemicals



- 1,2-Benzenedicarboxylic acid, monobutyl ester; 131-70-4
 - ► Hazardous Substances Data Bank (HSDB)
- 1,2-Benzenedicarboxylic acid, mono(phenylmethyl) ester; 2528-16-7
 - ▶ Hazardous Substances Data Bank (HSDB)

6 Chemical Vendors

? [2

PubChem

7 Food Additives and Ingredients

? [2

7.1 FDA Indirect Additives used in Food Contact Substances

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(:)	11

Indirect Additives	BUTYL BENZYL PHTHALATE
Title 21 of the U.S. Code of	175.105
	176.170
Federal Regulations (21 CFR)	176.180
CFR)	177.2420
	178.3740

[▶] FDA Center for Food Safety and Applied Nutrition (CFSAN)

8 Pharmacology and Biochemistry



8.1 MeSH Pharmacological Classification



Teratogens

An agent that causes the production of physical defects in the developing embryo. (See all compounds classified as Teratogens.)

Medical Subject Headings (MeSH)

8.2 Absorption, Distribution and Excretion



This study examined the extent of dermal absorption of a series of phthalate diesters in the rat. Those tested were dimethyl, diethyl, diisobutyl, and the area of application was covered with a perforated cap. The rat was restrained and housed for 7 days in a metabolic cage that allowed separate collection of urine and feces. Urine and feces were collected every 24 hr, and the amount of carbon-14 excreted was taken as an index of the percutaneous absorption. At 24 hr, diethyl phthalate showed the greatest excretion (26%). As the length of the alkyl side chain increased, the amount of carbon-14 excreted in the first 24 hr decreased significantly. The cumulative percentage dose excreted in 7 days was greatest for diethyl, dibutyl, and diisobutyl phthalate, about 50-60% of the applied 14C; and intermediate (20-40%) for dimethyl, benzyl butyl, and dihexyl phthalate. Urine was the major route of excretion of all phthalate diesters except for diisodecyl phthalate. This compound was poorly absorbed and showed almost no urinary excretion. After 7 days, the percentage dose for each phthalate that remained in the body was minimal and showed no specific tissue distribution. Most of the unexcreted dose remained in the area of application. These data show that the structure of the phthalate diester determines the degree of dermal absorption. Absorption maximized with diethyl phthalate and then decreased significantly as the alkyl side chain length increased.

PMID:2925020

Elsisi AE et al; Fundam Appl Toxicol 12(1): 70-7 (1989)

▶ Hazardous Substances Data Bank (HSDB)

... Male Fischer-344 rats were dosed with (14)C-labeled butyl benzyl phthalate (BBP) at 2, 20, 200, or 2000 mg/kg orally or 20 mg/kg iv to detect the effects of dose on rates and routes of excretion. In 24 hr, 61-74% of the dose was excreted in the urine and 13-19% in the feces at 2-200 mg/kg. At 2000-mg/kg, 16% of the (14)C was excreted in the urine and 57% in the feces. Urinary (14)C was composed of monophthalate glucuronides derivatives (MP: 10-42% of the dose) and monophthalate glucuronides (2-21% of the dose). At 4 hr after iv administration of BBP (20 mg/kg), 53-58% of the dose was excreted in the bile of anesthetized rats. BBP was not found in the bile, but monobutyl glucuronide and monobenzyl phthalate glucuronide (26 and 13% of the dose, respectively) and trace amts of free monoesters (2% of the dose) and unidentified metabolites (14% of the dose) were present. ... The half-lives of BBP, MP, and total (14)C in blood (20 mg/kg, iv) were 10 min, 5.9 hr, and 6.3 hr, respectively. ...

PMID:3959124

Eigenberg DA et al; J Toxicol Environ Health 17 (4): 445-56 (1986)

▶ Hazardous Substances Data Bank (HSDB)

Following intravenous administration of 20 mg/kg of (14)C-BBP, 55% of the dose was excreted into bile and 34% was excreted into the urine.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 869

▶ Hazardous Substances Data Bank (HSDB)

Beagle dogs were given a 5 g/kg bw oral dose of butyl benzyl phthalate divided over a 4 hr period. Unchanged butyl benzyl phthalate in the feces comprised 88-91% of the dose. While butyl benzyl phthalate was not present in the urine, some 4.2% of the dose was present as phthalic acid

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: https://monographs.iarc.fr/ENG/Classification/index.php, p. V73 119 (1999)

▶ Hazardous Substances Data Bank (HSDB)

For more Absorption, Distribution and Excretion (Complete) data for BUTYL BENZYL PHTHALATE (8 total), please visit the HSDB record page.

▶ Hazardous Substances Data Bank (HSDB)

8.3 Metabolism/Metabolites





BBP was not found in the bile, but monobutyl glucuronide and monobenzyl phthalate glucuronide (26 and 13% of the dose, respectively) and trace amounts of free monoesters (2% of the dose) and unidentified metabolites (14% of the dose) were present. Although BBP is an asymetrical diester with the potential of forming equal amounts of monobutyl phthalate and monobenzyl phthalate, larger quantities of monobutyl phthalate were formed (monobutyl phthalate= 44% vs monobenzyl phthalate= 16% of the dose). ...

PMID:3959124

Eigenberg DA et al; J Toxicol Environ Health 17 (4): 445-56 (1986)

▶ Hazardous Substances Data Bank (HSDB)

The urinary monoester metabolites of seven commonly used phthalates /were measured/ in approximately 2,540 samples collected from participants of the National Health and Nutrition Examination Survey (NHANES), 1999-2000, who were greater than or equal to 6 years of age. ... Detectable levels of metabolites monoethyl phthalate (MEP), monobutyl phthalate (MBP), monobenzyl phthalate (MBZP), and mono-(2ethylhexyl) phthalate (MEHP) /were found/ in > 75% of the samples, suggesting widespread exposure in the United States to diethyl phthalate, dibutyl phthalate or diisobutylphthalate, benzylbutyl phthalate, and di-(2-ethylhexyl) phthalate, respectively. ... Monoisononyl phthalate, mono-cyclohexyl phthalate, and mono-n-octyl phthalate /were detected infrequently/, suggesting that human exposures to di-isononyl phthalate, dioctylphthalate, and dicyclohexyl phthalate, respectively, are lower than those listed above, or the pathways, routes of exposure, or pharmacokinetic factors such as absorption, distribution, metabolism, and elimination are different. Non-Hispanic blacks had significantly higher concentrations of MEP than did Mexican Americans and non-Hispanic whites. Compared with adolescents and adults, children had significantly higher levels of MBP, MBzP, and MEHP but had significantly lower concentrations of MEP. Females had significantly higher concentrations of MEP and MBzP than did males, but similar MEHP levels. Of particular interest, females of all ages had significantly higher concentrations of the reproductive toxicant MBP than did males of all ages; however, women of reproductive age (i.e., 20-39 years of age) had concentrations similar to adolescent girls and women 40 years of age...

PMID:14998749

Full text: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC1241863

Silva MJ et al; Environ Health Perspect 112 (3): 331-8 (2004); Erratum in: Environ Health Perspect 112 (5): A270 (2004).

▶ Hazardous Substances Data Bank (HSDB)

Three groups of eight volunteers were administered stable isotope-labelled ... benzylbutylphthalate. ... For benzylbutylphthalate, 67% and 78% was eliminated as monobenzylphthalate and only 6% (measured for the high dose only) was eliminated as monobutylphthalate. ...

PMID:11761117

Anderson WA et al; Food Addit Contam 18 (12): 1068-74 (2001)

Hazardous Substances Data Bank (HSDB)

n-Butyl benzyl phthalate (BBP) ... has been orally administered to female Wistar rats with four doses (150, 475, 780 and 1500 mg/kg body weight/day) for 3 consecutive days. Metabolites recovered in urine were analyzed by gas chromatography-mass spectrometry (GC-MS) after 24, 48 and 72 hours. Six metabolites were identified. Mono-n-butyl phthalate (MBuP) and mono-n-benzyl phthalate (MBeP) represented respectively 29-34% and 7-12% of the total recovered metabolites. Hippuric acid, the main metabolite of benzoic acid, represented the second major metabolite (51-56%). Phthalic acid, benzoic acid and an omega-oxidized metabolite of MBuP were also recovered in urine but in small quantities. BBP was never identified in urine. Total urinary metabolites recovery represented 56% of the dose administered in the first 24 hours. However, total recovery decreased when the dose increases (43% at 780 mg/kg body weight/day, only 30% at 1500 mg/kg body weight/day). Whatever the time was, BBP metabolites recovered in urine were all present and in the same proportions for the two lowest doses. Discrepancy in metabolites quantities expressed as percentages of the dose observed in urine of rat treated with the highest BBP dose disappeared with time as MBuP, MBeP and hippuric acid recovery has significantly increased at day 3. ...

PMID:10506015

Nativelle C et al; Food Chem Toxicol 37 (8): 905-17 (1999)

Hazardous Substances Data Bank (HSDB)

For more Metabolism/Metabolites (Complete) data for BUTYL BENZYL PHTHALATE (9 total), please visit the HSDB record page.

8.4 Biological Half-Life



Fish Biotrans. Half-Life (Km)

0.09 Days

▶ EPA DSSTox

The half-lives of butyl benzyl phthalate (BBP), monophthalate (MP), and total (14)C in blood (20 ng/kg, intravenously) were 10 min, 5.9 hr, and 6.3 hr, respectively.

Eigenberg DA et al; J Toxicol Environ Health 17 (4): 445-56 (1986)

▶ Hazardous Substances Data Bank (HSDB)

The half-life of BBP in blood is 10 min following an oral administration of 5 g/kg to dogs.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 869

9 Use and Manufacturing	
9.1 Use Classification	② Z
Health Hazards -> Carcinogens	
NJDOH RTK Hazardous Substance List	
9.2 Household Products	② Z
Household & Commercial/Institutional Products	
Information on 55 consumer products that contain Butyl benzyl phthalate in the following categories is provided:	
• Auto Products	
• Hobby/Craft	
Home Maintenance	
• Inside the Home	
• Landscaping/Yard	
Consumer Product Information Database (CPID)	

EPA CPDat Chemical and Product Categories

9.3 Uses

The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products, Scientific Data, volume 5, Article number: 180125 (2018), DOI:10.1038/sdata.2018.125

▶ EPA Chemical and Products Database (CPDat)

PLASTICIZER FOR PVC-BASED FLOORING PRODUCTS, POLYVINYL ACETATE EMULSION ADHESIVES, OTHER PLASTICS, EG, ETHYL CELLULOSE, IN COATINGS, EG, FOR AUTOMOBILES

SRI

▶ Hazardous Substances Data Bank (HSDB)

Plasticizer for polyvinyl and cellulose resins, organic intermediate.

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 196

▶ Hazardous Substances Data Bank (HSDB)

It is used as a plasticizer for polyvinyl chloride plastics, particularly vinyl floor tile, vinyl leather, and cloth coating. It may be used in sealants, foams, adhesives, coating and inks, car care products, and cosmetics.

David RM et al; Esters of Mono-, Di-, and Tricarboxylic Acids. Patty's Toxicology. 6th ed. (1999-2015). New York, NY: John Wiley & Sons, Inc. On-line Posting Date: 17 Aug 2012

▶ Hazardous Substances Data Bank (HSDB)

Congress has permanently banned three types of phthalates (DEHP, DBP, BBP) in any amount greater than 0.1 percent (computed for each phthalate, individually) in (1) children's toys and (2) certain child care articles. /Di-(2-ethylhexyl) phthalate (DEHP), dibutyl phthalate (DBP), or benzyl butyl phthalate (BBP)/

US CPSC; Phthalates; Available from, as of March 11, 2015: https://www.cpsc.gov/en/Business--Manufacturing/Business-Education/Business-Guidance/Phthalates-Information/

▶ Hazardous Substances Data Bank (HSDB)

9.3.1 Industry Uses

② [2

Fillers

Plasticizers

https://www.epa.gov/chemical-data-reporting

▶ EPA Chemicals under the TSCA

9.3.2 Consumer Uses



Adhesives and sealants

Floor coverings

Paints and coatings

https://www.epa.gov/chemical-data-reporting

▶ EPA Chemicals under the TSCA

9.4 Methods of Manufacturing



... First synthesized by the reaction of the monobutyl ester of phthalic acid with benzyl chloride in neutral aqueous or alcoholic solution. Commercial production in the USA based on the same process with the monobutyl ester produced by the reaction of phthalic anhydride with n-butyl alcohol in the presence of an acidic catalyst. In Japan, the monobutyl ester is treated with benzyl alcohol in the presence of an acidic catalyst.

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: https://monographs.iarc.fr/ENG/Classification/index.php, p. V29 194 (1982)

▶ Hazardous Substances Data Bank (HSDB)

BBP is manufactured via by the sequential addition of butanol and benzyl chloride to phthalic anhydride.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 867

▶ Hazardous Substances Data Bank (HSDB)

9.5 Formulations/Preparations



Grade: Technical.

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 196

▶ Hazardous Substances Data Bank (HSDB)

9.6 U.S. Production

Aggregated Product Volume (EPA CDR 2016)

10,000,000 - 50,000,000 lb

https://www.epa.gov/chemical-data-reporting

▶ EPA Chemicals under the TSCA

(1977) 6.81X10+10 G

SRI

▶ Hazardous Substances Data Bank (HSDB)

(1981) 7.47X10+10 G

SRI

▶ Hazardous Substances Data Bank (HSDB)

Over 100 million pounds of butyl benzyl phthalate (BBP) were produced in 1978.

Gledhill WE et al; Env Sci Tech 14: 301-5 (1980)

▶ Hazardous Substances Data Bank (HSDB)

Production volumes for non-confidential chemicals reported under the Inventory Update Rule.

Year	Production Range (pounds)
1986	>50 million - 100 million
1990	>100 million - 500 million
1994	>50 million - 100 million
1998	>100 million - 500 million
2002	>50 million - 100 million

US EPA; Non-confidential Production Volume Information Submitted by Companies for Chemicals Under the 1986-2002 Inventory Update Rule (IUR). 1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester (85-68-7). Available from, as of April 22, 2008: https://www.epa.gov/oppt/iur/tools/data/2002-vol.html

▶ Hazardous Substances Data Bank (HSDB)

For more U.S. Production (Complete) data for BUTYL BENZYL PHTHALATE (7 total), please visit the HSDB record page.

9.7 General Manufacturing Information



Industry Processing Sectors

Adhesive manufacturing Custom compounding of purchased resin Plastics product manufacturing

▶ EPA Chemicals under the TSCA

EPA TSCA Commercial Activity Status

1,2-Benzenedicarboxylic acid, 1-butyl 2-(phenylmethyl) ester: ACTIVE

https://www.epa.gov/tsca-inventory

▶ EPA Chemicals under the TSCA

A gas-permeable contact lens composition consisted of a partially esterified cellulose polymer and a compatible plasticizer /including butyl benzyl phthalate/ in an amount sufficient to incr the oxygen permeability of the cellulose polymer greater than or equal to 13% higher than that of the unplasticized polymer.

CONTACT LENSES; BRIT UK PAT APPL PATENT NO 1593553 07/15/81 (WESLEY-JESSEN, INC)

▶ Hazardous Substances Data Bank (HSDB)

Congress has permanently banned three types of phthalates (DEHP, DBP, BBP) in any amount greater than 0.1 percent (computed for each phthalate, individually) in (1) children's toys and (2) certain child care articles. /Di-(2-ethylhexyl) phthalate (DEHP), dibutyl phthalate (DBP), or benzyl butyl phthalate (BBP)/

US CPSC; Phthalates; Available from, as of March 11, 2015: https://www.cpsc.gov/en/Business--Manufacturing/Business-Education/Business-Guidance/Phthalates-Information/

▶ Hazardous Substances Data Bank (HSDB)

9.8 Sampling Procedures





Two methods for the collection of ambient organic vapors (potential toxic and carcinogenic compounds) at the ng/cu m to ug/cu m level were utilized in field sampling at a residential site in Portland (Oregon, USA) during the winter and spring of 1984. The methods were adsorption/solvent extraction with polyurethane foam plugs (ASE/PUFP) and adsorption/thermal desorption with Tenax-GC cartridges (ATD/Tenax-GC). ASE/PUFP was used with a single sample flow rate in a single channel of the sampler. ATD/Tenax-GC was used with 2 different sample flow rates in 2 separate channels. Each method was well suited to the analysis of compounds in a specific range of volatility. ... The low sample volumes used with ATD/Tenax-GC for determinations at the ng/cu m level make it an attractive method for many applications.

Ligocki MP, Pankow JF; Anal Chem 57 (6): 1138-44 (1985)

10 Identification



10.1 Analytic Laboratory Methods



Method: DOE OM100R; Procedure: gas chromatography with mass spectrometer ion trap detector; Analyte: butyl benzyl phthalate; Matrix: solid waste matrices, soils, and groundwater; Detection Limit: 76 ug/L.

National Environmental Methods Index; Analytical, Test and Sampling Methods. Butyl Benzyl Phthalate (85-68-7). Available from, as of March 4, 2015: https://www.nemi.gov

▶ Hazardous Substances Data Bank (HSDB)

Method: EPA-EAD 1625; Procedure: gas chromatography/mass spectrometry; Analyte: butyl benzyl phthalate; Matrix: water; Detection Limit: not provided.

National Environmental Methods Index: Analytical. Test and Sampling Methods. Butyl Benzyl Phthalate (85-68-7). Available from, as of March 4, 2015: https://www.nemi.gov

▶ Hazardous Substances Data Bank (HSDB)

Method: EPA-EAD 606; Procedure: gas chromatography with electron capture detector; Analyte: butyl benzyl phthalate; Matrix: wastewater and other waters; Detection Limit: 0.34 ug/L.

National Environmental Methods Index; Analytical, Test and Sampling Methods. Butyl Benzyl Phthalate (85-68-7). Available from, as of March 4, 2015: https://www.nemi.gov

▶ Hazardous Substances Data Bank (HSDB)

Method: EPA-NERL 506; Procedure: gas chromatography with photoionization detection; Analyte: butyl benzyl phthalate; Matrix: drinking water; Detection Limit: 2.67 ug/L.

National Environmental Methods Index; Analytical, Test and Sampling Methods. Butyl Benzyl Phthalate (85-68-7). Available from, as of March 4, 2015: https://www.nemi.gov

▶ Hazardous Substances Data Bank (HSDB)

For more Analytic Laboratory Methods (Complete) data for BUTYL BENZYL PHTHALATE (13 total), please visit the HSDB record page.

▶ Hazardous Substances Data Bank (HSDB)

10.2 Clinical Laboratory Methods



We have developed a gas chromatography-mass spectrometry (GC-MS) method to determine five phthalate monoesters (monoethyl phthalate (MEP), mono-n-butyl phthalate (MBP), mono-(2-ethylhexyl) phthalate (MINP) and monobenzyl phthalate (MBZ)) in human urine. Human urine samples were subjected to enzymatic deconjugation of the glucuronides followed by extraction with hexane. The extracted phthalate monoesters were methylated with diazomethane, purified on a Florisil column and then subjected to GC-MS analysis. The recoveries from urine spiked with five phthalate monoesters were 86.3%-119% with coefficients of variation of 0.6%-6.1%. We measured phthalate monoester levels in human urine by analyzing 36 samples from volunteers. MBP and MEP were detected in all samples, and their median concentrations were 60.0 and 10.7 ng/mL, respectively. MBzP and MEHP were found in 75% and 56% of samples, and their median concentrations were 10.9 and 5.75 ng/mL, respectively. MINPs were not detected in most samples (6% detectable). Women had significantly (p < 0.05) higher mean concentrations of MBP and MEP than men. The estimated daily exposure levels for the four parent phthalates excluding diisononyl phthalate ranged from 0.27 to 5.69 mug/kg/day (median).

PMID:20574658

Kondo F et al; Bull Environ Contam Toxicol. 85 (1): 92-6 (2010)

▶ Hazardous Substances Data Bank (HSDB)

A cleanup of biological samples is described: phthalate plasticizers are quantitated by gas chromatography, confirmed by measurement of fluorescense in concn sulfuric acid. /Phthalate plasticizers/

11 Safety and Hazards 11.1 Hazards Identification 11.1.1 GHS Classification Showing 1 of 7 View More Pictogram(s) Health Hazard Signal Danger H360Df: May damage the unborn child; Suspected of damaging fertility [Danger Reproductive toxicity] **GHS Hazard Statements** H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard] H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard] P201, P202, P273, P281, P308+P313, P391, P405, and P501 **Precautionary Statement** Codes (The corresponding statement to each P-code can be found at the GHS Classification page.)

▶ EU REGULATION (EC) No 1272/2008

11.1.2 Hazard Classes and Categories

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Showing 2 of 6 View More

Repr. 1B

Aquatic Acute 1

Aquatic Chronic 1

▶ EU REGULATION (EC) No 1272/2008

Repr. 1B (100%)

Aquatic Acute 1 (99.91%)
Aquatic Chronic 1 (100%)

▶ European Chemicals Agency (ECHA)

11.1.3 NFPA Hazard Classification



NFPA 704 Diamond



NFPA Health Rating

1 - Materials that, under emergency conditions, can cause significant irritation.

NFPA Fire Rating	1 - Materials that must be preheated before ignition can occur. Materials require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur.
NFPA Instability Rating	0 - Materials that in themselves are normally stable, even under fire conditions.

11.1.4 Substance of Very High Concern (SVHC)



REACH Restricted Substance

Restricted substance: Benzyl butyl phthalate (BBP) Restriction condition document: PDF link

▶ European Chemicals Agency (ECHA)

REACH SVHC Substance

Substance: Benzyl butyl phthalate (BBP)

Reason: Toxic for reproduction (Article 57c), Endocrine disrupting properties (Article 57(f) - human health)

Decision Document1: PDF Link Decision Document2: PDF Link Decision Document3: PDF Link

▶ European Chemicals Agency (ECHA)

11.1.5 Health Hazards



Prolonged contact with liquid causes some irritation of eyes and skin. (USCG, 1999)

U.S. Coast Guard. 1999. Chemical Hazard Response Information System (CHRIS) - Hazardous Chemical Data. Commandant Instruction 16465.12C. Washington, D.C.: U.S. Government Printing Office.

CAMEO Chemicals

Carcinogens

NJDOH RTK Hazardous Substance List

11.1.6 Fire Hazards



Special Hazards of Combustion Products: Irritating vapors of unburned chemical may form in fires. (USCG, 1999)

U.S. Coast Guard. 1999. Chemical Hazard Response Information System (CHRIS) - Hazardous Chemical Data. Commandant Instruction 16465.12C. Washington, D.C.: U.S. Government Printing Office.

CAMEO Chemicals

Combustible. Gives off irritating or toxic fumes (or gases) in a fire.

▶ ILO International Chemical Safety Cards (ICSC)

11.1.7 Fire Potential



Combustible

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 196

▶ Hazardous Substances Data Bank (HSDB)

11.1.8 Skin, Eye, and Respiratory Irritations

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Irritates the eyes, the skin, and the respiratory tract.

Pohanish, R.P. (ed). Sittig's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K, Volume 2: L-Z. William Andrew, Waltham, MA 2012, p. 467

▶ Hazardous Substances Data Bank (HSDB)

11.2 Safety and Hazard Properties



11.2.1 Lower Explosive Limit (LEL)



1.2 % at 451° F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

11.3 First Aid Measures



11.3.1 First Aid



EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop. SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. IMMEDIATELY call a hospital or poison control center even if no symptoms (such as redness or irritation) develop. IMMEDIATELY transport the victim to a hospital for treatment after washing the affected areas. INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. IMMEDIATELY call a physician and be prepared to transport the victim to a hospital even if no symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing. INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital. OTHER: Since this chemical is a known or suspected carcinogen you should contact a physician for advice regarding the poss

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

11.3.2 Inhalation First Aid



Fresh air, rest.

▶ ILO International Chemical Safety Cards (ICSC)

 -	20.12), 24.9, P.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1	
1.3.3 Skin First Aid		② Z
Remove contaminated clothes. Rinse and then wash skin with water and soap.		
▶ ILO International Chemical Safety Cards (ICSC)		
		_
1.3.4 Eye First Aid		? Z
First rinse with plenty of water for several minutes (remove contact lenses if easily possible)), then refer for medical attention.	
▶ ILO International Chemical Safety Cards (ICSC)		
1.3.5 Ingestion First Aid		? Z
Rinse mouth.		
▶ ILO International Chemical Safety Cards (ICSC)		

11.4 Fire Fighting

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Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]: SMALL FIRE: Dry chemical, CO2, water spray or regular foam. LARGE FIRE: Water spray, fog or regular foam. Do not scatter spilled material with high-pressure water streams. Move containers from fire area if you can do it without risk. Dike fire-control water for later disposal. FIRE INVOLVING TANKS: Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. (ERG, 2016)

U.S. Department of Transportation, Transport Canada, and Secretariat of Communications and Transport of Mexico, with collaboration from Argentina's Centro de Información Química para Emergencias. 2016 Emergency Response Guidebook. https://www.phmsa.dot.gov/hazmat/outreach-training/erg (accessed April 26, 2016).

CAMEO Chemicals

Use alcohol-resistant foam, powder, carbon dioxide, water spray.

▶ ILO International Chemical Safety Cards (ICSC)

11.4.1 Fire Fighting Procedures



To fight fire, use spray or mist, carbon dioxide, dry chemical.

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 401

▶ Hazardous Substances Data Bank (HSDB)

Water may cause frothing. Use dry chemical, carbon dioxide, or foam extinguishers.

Pohanish, R.P. (ed). Sittig's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K,Volume 2: L-Z. William Andrew, Waltham, MA 2012, p. 468

▶ Hazardous Substances Data Bank (HSDB)

From a secure, explosion-proof location, use water spray to cool exposed containers. If cooling streams are ineffective (venting sound increases in volume and pitch, tank discolors, or shows any signs of deforming), withdraw immediately to a secure position.

Pohanish, R.P. (ed). Sittig's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K,Volume 2: L-Z. William Andrew, Waltham, MA 2012, p. 468

If material involved in fire: Extinguish fire using agent suitable for type of surrounding fire (Material itself does not burn or burns with difficulty.). Use dry chemical or carbon dioxide. Keep run-off water out of sewers and water sources.

Association of American Railroads; Bureau of Explosives. Emergency Handling of Hazardous Materials in Surface Transportation. Association of American Railroads, Pueblo, CO. 2005, p. 147

▶ Hazardous Substances Data Bank (HSDB)

For more Fire Fighting Procedures (Complete) data for BUTYL BENZYL PHTHALATE (7 total), please visit the HSDB record page.

▶ Hazardous Substances Data Bank (HSDB)

11.4.2 Firefighting Hazards

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Poisonous gases are produced in fire.

Pohanish, R.P. (ed). Sittia's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K, Volume 2: L-Z. William Andrew, Waltham, MA 2012, p. 468

▶ Hazardous Substances Data Bank (HSDB)

11.5 Accidental Release Measures



11.5.1 Isolation and Evacuation



Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]: As an immediate precautionary measure, isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids. SPILL: Increase, in the downwind direction, as necessary, the isolation distance shown above. FIRE: If tank, rail car or tank truck is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2016)

U.S. Department of Transportation, Transport Canada, and Secretariat of Communications and Transport of Mexico, with collaboration from Argentina's Centro de Información Química para Emergencias. 2016 Emergency Response Guidebook. https://www.phmsa.dot.gov/hazmat/outreach-training/erg (accessed April 26, 2016).

CAMEO Chemicals

11.5.2 Spillage Disposal



Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

▶ ILO International Chemical Safety Cards (ICSC)

11.5.3 Cleanup Methods



Environmental considerations-land spill: Dig a pit, pond, lagoon, holding area to contain liquid or solid material. Dike surface flow using soil, sand bags, foamed polyurethane, or foamed concrete. Absorb bulk liquid with fly ash, cement powder, or commercial sorbents. /SRP: If time permits, pits, ponds, lagoons, soak holes, or holding areas should be sealed with an impermeable flexible membrane liner./

Association of American Railroads; Bureau of Explosives. Emergency Handling of Hazardous Materials in Surface Transportation. Association of American Railroads, Pueblo, CO. 2005, p. 147

▶ Hazardous Substances Data Bank (HSDB)

Environmental considerations-water spill: Use natural barriers or oil spill control booms to limit spill travel. Remove trapped material with suction hoses.

Association of American Railroads; Bureau of Explosives. Emergency Handling of Hazardous Materials in Surface Transportation. Association of American Railroads, Pueblo, CO. 2005, p. 147

Environmental considerations-air spill: Apply water spray or mist to knock down vapors.

Association of American Railroads; Bureau of Explosives. Emergency Handling of Hazardous Materials in Surface Transportation. Association of American Railroads, Pueblo, CO. 2005, p. 147

▶ Hazardous Substances Data Bank (HSDB)

ACCIDENTAL RELEASE MEASURES Personal precautions, protective equipment and emergency procedures Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. For personal protection see section Environmental precautions Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided. Methods and materials for containment and cleaning up Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

Sigma-Aldrich; Material Safety Data Sheet for Benzyl butyl phthalate, Product Number: 308501, Version 5.4 (Revision Date 01/02/2015). Available from, as of March 11, 2015: https://www.sigmaaldrich.com/safety-center.html

▶ Hazardous Substances Data Bank (HSDB)

11.5.4 Disposal Methods





SRP: Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in air, soil or water; effects on animal, aquatic and plant life; and conformance with environmental and public health regulations. If it is possible or reasonable use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination.

▶ Hazardous Substances Data Bank (HSDB)

Incineration: It should be atomized into an incinerator and combustion may be improved by mixing with a more flammable solvent (acetone or benzene).

United Nations. Treatment and Disposal Methods for Waste Chemicals (IRPTC File). Data Profile Series No. 5. Geneva, Switzerland: United Nations Environmental Programme, Dec. 1985., p. 258

▶ Hazardous Substances Data Bank (HSDB)

Product Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Contaminated packaging Dispose of as unused product.

Sigma-Aldrich; Material Safety Data Sheet for Benzyl butyl phthalate, Product Number: 308501, Version 5.4 (Revision Date 01/02/2015). Available from, as of March 11, 2015: https://www.sigmaaldrich.com/safety-center.html

▶ Hazardous Substances Data Bank (HSDB)

11.5.5 Preventive Measures



SRP: The scientific literature for the use of contact lenses by industrial workers is inconsistent. The benefits or detrimental effects of wearing contact lenses depend not only upon the substance, but also on factors including the form of the substance, characteristics and duration of the exposure, the uses of other eye protection equipment, and the hygiene of the lenses. However, there may be individual substances whose irritating or corrosive properties are such that the wearing of contact lenses would be harmful to the eye. In those specific cases, contact lenses should not be worn. In any event, the usual eye protection equipment should be worn even when contact lenses are in place.

▶ Hazardous Substances Data Bank (HSDB)

If material not involved in fire: Keep material out of water sources and sewers. Build dikes to contain flow as necessary.

Association of American Railroads; Bureau of Explosives. Emergency Handling of Hazardous Materials in Surface Transportation. Association of American Railroads, Pueblo, CO. 2005, p. 147

▶ Hazardous Substances Data Bank (HSDB)

Personnel protection: Keep upwind. Avoid breathing vapors.

Association of American Railroads; Bureau of Explosives. Emergency Handling of Hazardous Materials in Surface Transportation. Association of American Railroads, Pueblo, CO. 2005, p. 147

SRP: Contaminated protective clothing should be segregated in a manner such that there is no direct personal contact by personnel who handle, dispose, or clean the clothing. The completeness of the cleaning procedures should be considered before the decontaminated protective clothing is returned for reuse by the workers. Contaminated clothing should not be taken home at the end of shift, but should remain at employee's place of work for cleaning.

▶ Hazardous Substances Data Bank (HSDB)

For more Preventive Measures (Complete) data for BUTYL BENZYL PHTHALATE (8 total), please visit the HSDB record page.

▶ Hazardous Substances Data Bank (HSDB)

11.6 Handling and Storage



11.6.1 Nonfire Spill Response



Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]: Do not touch or walk through spilled material. Stop leak if you can do it without risk. Prevent dust cloud. Avoid inhalation of asbestos dust. SMALL DRY SPILL: With clean shovel, place material into clean, dry container and cover loosely; move containers from spill area. SMALL SPILL: Pick up with sand or other non-combustible absorbent material and place into containers for later disposal. LARGE SPILL: Dike far ahead of liquid spill for later disposal. Cover powder spill with plastic sheet or tarp to minimize spreading. Prevent entry into waterways, sewers, basements or confined areas. (ERG, 2016)

U.S. Department of Transportation, Transport Canada, and Secretariat of Communications and Transport of Mexico, with collaboration from Argentina's Centro de Información Química para Emergencias. 2016 Emergency Response Guidebook. https://www.phmsa.dot.gov/hazmat/outreach-training/erg (accessed April 26, 2016).

CAMEO Chemicals

11.6.2 Safe Storage



Store in an area without drain or sewer access. Separated from strong oxidants.

▶ ILO International Chemical Safety Cards (ICSC)

11.6.3 Storage Conditions



Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Storage class (TRGS 510): Non-combustible, acute toxic Cat.3 / toxic hazardous materials or hazardous materials causing chronic effects

Sigma-Aldrich; Material Safety Data Sheet for Benzyl butyl phthalate, Product Number: 308501, Version 5.4 (Revision Date 01/02/2015). Available from, as of March 11, 2015: https://www.sigmaaldrich.com/safety-center.html

▶ Hazardous Substances Data Bank (HSDB)

Store in tightly closed containers in a cool, well-ventilated area away from incompatible materials. Metal containers involving the transfer of this chemical should be grounded and bonded. Drums must be equipped with self-closing valves, pressure vacuum bungs, and flame arresters. Use only nonsparkling tools and equipment, especially when opening and closing containers of this chemical. Sources of ignition such as smoking and open flames are prohibited this chemical is used, handled, or stored in a manner that could create a potential fire or explosion hazard.

Pohanish, R.P. (ed). Sittia's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K, Volume 2: L-Z. William Andrew, Waltham, MA 2012, p. 468

▶ Hazardous Substances Data Bank (HSDB)

11.7 Exposure Control and Personal Protection





11.7.1 Threshold Limit Values (TLV)

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(inhalable fraction): 20 mg/m3; peak limitation category: II(2); pregnancy risk group: C

▶ ILO International Chemical Safety Cards (ICSC)

11.7.2 Other Standards Regulations and Guidelines



(a) Prohibition on the sale of certain products containing phthalates. Beginning on the date that is 180 days after the date of enactment of this Act, it shall be unlawful for any person to manufacture for sale, offer for sale, distribute in commerce, or import into the United States any children's toy or child care article that contains concentrations of more than 0.1 percent of di-(2-ethylhexyl) phthalate (DEHP), dibutyl phthalate (DBP), or benzyl butyl phthalate (BBP).

Consumer Prduct Safety Improvement Act of 2008. Section 108, Public Law 110-314 August 14, 2008. Available from, as of March 24, 2015: https://www.cpsc.gov/PageFiles/129663/cpsia.pdf

▶ Hazardous Substances Data Bank (HSDB)

11.7.3 Inhalation Risk



Evaporation at 20 °C is negligible; a harmful concentration of airborne particles can, however, be reached quickly on spraying.

▶ ILO International Chemical Safety Cards (ICSC)

11.7.4 Effects of Long Term Exposure



Animal tests show that this substance possibly causes toxicity to human reproduction or development.

ILO International Chemical Safety Cards (ICSC)

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11.7.5 Personal Protective Equipment (PPE)



Protective gloves and goggles (USCG, 1999)

U.S. Coast Guard. 1999. Chemical Hazard Response Information System (CHRIS) - Hazardous Chemical Data. Commandant Instruction 16465.12C. Washington, D.C.: U.S. Government Printing Office.

CAMEO Chemicals

Protective gloves and goggles.

U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5.

▶ Hazardous Substances Data Bank (HSDB)

Wear protective gloves and clothing to prevent any reasonable probability of skin contact. ... All protective clothing (suits, gloves, footwear, headgear) should be clean, available each day, and put on before work. ... Wear splash-proof chemical goggles and face shield unless full facepiece respiratory protection is worn. Employees should wash immediately with soap when skin is wet or contaminated. Provide emergency showers and eyewash.

Pohanish, R.P. (ed). Sittig's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K, Volume 2: L-Z. William Andrew, Waltham, MA 2012, p. 468

▶ Hazardous Substances Data Bank (HSDB)

Personnel protection: Wear appropriate chemical protective gloves, boots and goggles.

Association of American Railroads; Bureau of Explosives. Emergency Handling of Hazardous Materials in Surface Transportation. Association of American Railroads, Pueblo, CO. 2005, p. 147

Skin protection Handle with glov	Skin	n protection	Handle	with	alove
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Sigma-Aldrich; Material Safety Data Sheet for Benzyl butyl phthalate, Product Number: 308501, Version 5.4 (Revision Date 01/02/2015). Available from, as of March 11, 2015: https://www.sigmaaldrich.com/safety-center.html

▶ Hazardous Substances Data Bank (HSDB)

For more Personal Protective Equipment (PPE) (Complete) data for BUTYL BENZYL PHTHALATE (7 total), please visit the HSDB record page.

▶ Hazardous Substances Data Bank (HSDB)

11.7.6 Fire Prevention

NO open flames.

▶ ILO International Chemical Safety Cards (ICSC)

11.7.7 Exposure Prevention

② 🗹

See EFFECTS OF LONG-TERM OR REPEATED EXPOSURE. PREVENT GENERATION OF MISTS! AVOID EXPOSURE OF (PREGNANT) WOMEN!

▶ ILO International Chemical Safety Cards (ICSC)

11.7.8 Inhalation Prevention

② Z

Use ventilation, local exhaust or breathing protection.

▶ ILO International Chemical Safety Cards (ICSC)

11.7.9 Skin Prevention

②

Protective gloves.

▶ ILO International Chemical Safety Cards (ICSC)

11.7.10 Eye Prevention

② Z

Wear safety spectacles.

▶ ILO International Chemical Safety Cards (ICSC)

11.7.11 Ingestion Prevention

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Do not eat, drink, or smoke during work.

▶ ILO International Chemical Safety Cards (ICSC)

11.8 Stability and Reactivity	② Z
11.8.1 Air and Water Reactions	? Z
Slightly soluble in water and slightly denser than water.	
CAMEO Chemicals	
11.8.2 Reactive Group	⑦ Z
Esters, Sulfate Esters, Phosphate Esters, Thiophosphate Esters, and Borate Esters	
CAMEO Chemicals	
11.8.3 Reactivity Profile	? Z
BUTYL BENZYL PHTHALATE is an ester. Esters react with acids to liberate heat along with alcohols and acids. Strong oxidizing acids may cause a vigorous reaction that is sufficiently products. Heat is also generated by the interaction of esters with caustic solutions. Flammable hydrogen is generated by mixing esters with alkali metals and hydrides. Can generated Chemicals Safely 1980. p. 250].	
CAMEO Chemicals	
11.8.4 Hazardous Reactivities and Incompatibilities	? Z
Incompatible with strong acids, nitrates, oxidizers. Pohanish, R.P. (ed). Sittig's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K,Volume 2: L-Z. William Andrew, Waltham, MA 2012, p. 467 Hazardous Substances Data Bank (HSDB)	
Destructive to rubber and paint. Pohanish, R.P. (ed). Sittig's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K, Volume 2: L-Z. William Andrew, Waltham, MA 2012, p. 467 Hazardous Substances Data Bank (HSDB)	
Strong oxidizing agents, Strong bases Sigma-Aldrich; Material Safety Data Sheet for Benzyl butyl phthalate, Product Number: 308501, Version 5.4 (Revision Date 01/02/2015). Available from, as of March 11, 2015: https://www.sigmaaldrich.com Hazardous Substances Data Bank (HSDB)	n/safety-center.html
11.9 Transport Information	② Z
11.9.1 DOT Label	② Z
Class 9	
CAMEO Chemicals	

11.9.2 Packaging and Labelling	? Z
Marine pollutant.	
▶ ILO International Chemical Safety Cards (ICSC)	
	□ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □
11.9.3 EC Classification	? 🛭
Symbol: T, N; R: 61-62-50/53; S: 45-53-60-61	
▶ ILO International Chemical Safety Cards (ICSC)	
11.9.4 UN Classification	② Z
UN Hazard Class: 9; UN Pack Group: III	
▶ ILO International Chemical Safety Cards (ICSC)	
	□ Γ ²
11.10 Regulatory Information	? Z
11.10.1 State Drinking Water Guidelines	? Z
(MN) MINNESOTA 100 ug/L	
USEPA/Office of Water; Federal-State Toxicology and Risk Analysis Committee (FSTRAC). Summary of State and Federal Drinking Water Standards and Guidelines (11/93) To Present	
Hazardous Substances Data Bank (HSDB)	
(FL) FLORIDA 140 ug/L	
USEPA/Office of Water; Federal-State Toxicology and Risk Analysis Committee (FSTRAC). Summary of State and Federal Drinking Water Standards and Guidelines (11/93) To Present	
▶ Hazardous Substances Data Bank (HSDB)	
11.10.2 CERCLA Reportable Quantities	? Z
Persons in charge of vessels or facilities are required to notify the National Response Center (NRC) immediately, when there is a release of this designated hazardous substance, in an amount equal to	or greater
than its reportable quantity of 100 lb or 45.4 kg. The toll free number of the NRC is (800) 424-8802. The rule for determining when notification is required is stated in 40 CFR 302.4 (section IV. D.3.b). 40 CFR 302.4 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 26, 2015: https://www.ecfr.gov	y
▶ Hazardous Substances Data Bank (HSDB)	
	♠ □
11.10.3 TSCA Requirements	② Z
Pursuant to section 8(d) of TSCA EPA promulagated a model Health and Safety Data Reporting Rule. The section 8(d) model rule requires manufacturers, importers, and processors of listed chemical	substances

Pursuant to section 8(d) of TSCA, EPA promulagated a model Health and Safety Data Reporting Rule. The section 8(d) model rule requires manufacturers, importers, and processors of listed chemical substances and mixtures to submit to EPA copies and lists of unpublished health and safety studies. Butyl benzyl phthalate is included on this list. Effective date 04/29/83; Sunset date 04/29/93.

40 CFR 716.120 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 26, 2015: https://www.ecfr.gov

11.10.4 FDA Requirements

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Butyl benzyl phthalate is an indirect food additive for use only as a component of adhesives.

21 CFR 175.105 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 26, 2015: https://www.ecfr.gov

▶ Hazardous Substances Data Bank (HSDB)

11.11 Other Safety Information

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11.11.1 Toxic Combustion Products



Carbon oxides

Sigma-Aldrich; Material Safety Data Sheet for Benzyl butyl phthalate, Product Number: 308501, Version 5.4 (Revision Date 01/02/2015). Available from, as of March 11, 2015: https://www.sigmaaldrich.com/safety-center.html

▶ Hazardous Substances Data Bank (HSDB)

11.11.2 Special Reports



DHHS/NTP-CERHR Monograph on the Potential Human Reproductive and Developmental Effects of Butyl Benzyl Phthalate (BBP) (2003) NIH Publication No. 03-4487. BBP is one of 7 phthalate chemicals evaluated by the NTP CERHR Phthalates Expert Panel. These phthalates were selected for evaluation because of high production volume, extent of human exposures, use in children's products, and/or published evidence of reproductive or developmental toxicity. NTP-CERHR monographs are transmitted to federal and state agencies, interested parties, and the public and are available in electronic PDF format on the CERHR web site and in printed text or CD-ROM from the CERHR.[Available from, as of May 20, 2008: http://cerhr.niehs.nih.gov]

▶ Hazardous Substances Data Bank (HSDB)

European Chemicals Bureau; IUCLID Robust Summaries & Test Plans: Phthalate Esters Category, Benzyl butyl phthalate (85-68-7) (2000 CD-ROM edition) contains information on use, toxicology, and environmental effects of this chemical as supplied to the European Union by industry.[Available from, as of May 20, 2008: http://esis.jrc.ec.europa.eu/]

▶ Hazardous Substances Data Bank (HSDB)

Pierce RC et al; Natl Res Counc Can Assoc Comm Sci Criter Environ Qual Publ 0(17583) 1-100 (1980) the Physical-chemical properties, analytical determination & environmental dynamics of phthalate esters (industrial plasticizers) are reviewed.

▶ Hazardous Substances Data Bank (HSDB)

Nat'l Research Council Canada; Phthalate Esters In The Aquatic Environment (1980) NRCC No. 17583

▶ Hazardous Substances Data Bank (HSDB)

For more Special Reports (Complete) data for BUTYL BENZYL PHTHALATE (8 total), please visit the HSDB record page.

12 Toxicity

12.1 Toxicological Information

12.1.1 Toxicity Summary



IDENTIFICATION AND USE: Butyl benzyl phthalate (BBP) is a clear oily liquid that is used as a plasticizer mainly in polyvinyl chloride for vinyl floor tile, vinyl foams and carpet backing and in cellulose plastics and polyurethane. HUMAN EXPOSURE AND TOXICITY: BBP was not observed to be a primary irritant or sensitizer in skin patch tests with volunteers. Prenatal exposure to BBP may influence the risk of developing eczema in early childhood. BBP was also positively associated with airway inflammation in children. BBP was positive in E-Screen assay used to measure the proliferation of MCF-7 cells, a human breast cancer cell line. In another study proteomic changes in proteins secreted by human hepatocellular carcinomas (HepG2) cells exposed to BBP were evaluated. These proteins were found to be involved in apoptosis, signaling, tumor progression, energy metabolism, and cell structure and motility. BBP treatment of plasmacytoid DC cells suppressed IFN-gamma but enhanced IL-13 production by CD4+ T cells. ANIMAL STUDIES: The acute toxicity of this compound is low, with oral LD50 values in rats being greater than 2 g/kg body weight. Target organs following acute exposure include the hematological and central nervous systems. Repeated dose toxicity studies of this compound in the rat show decreases in body weight gain and increases in organ to body weight ratios, particularly for the kidney and liver. Histopathological effects on the pancreas and kidney and hematological effects have also been observed. At higher doses, degenerative effects on the testes and, occasionally histopathological effects on the liver have been reported. In specialized investigations, peroximal proliferation in the liver has been noted. The chronic toxicity and carcinogenicity of BBP bioassays in rats and mice, indicated that there was some evidence of carcinogenicity in male rats, based on an increased incidence of pancreatic tumors, and equivocal evidence in female rats, based on marginal increases in pancreatic and bladder tumors. Dietary restriction prevented full expression of the pancreatic tumors. There was no evidence for the carcinogenicity of BBP in mice. BBP is not genotoxic. In a range of studies, including those designed to investigate the reproductive effects of BBP on the testes and endocrine hormone in male rats, a modified mating protocol and a one generation study, adverse effects on the testes and, consequently fertility have generally been observed only at doses higher than those that induce effects on other organs (such as the kidney and liver), although decreases in sperm counts have been observed at doses similar to those that induce effects in the kidney and liver. Reduction in testes weight and daily sperm production in the offspring were reported at relatively low level in rats exposed in utero and during lactation. Neither BBP nor its principal metabolites have been uteritrophic in vivo in rats or mice, In several well conducted studies in rats and mice, butyl benzyl phthalate induced marked developmental effects, but only at dose levels that induce significant maternal toxicity. BBP administration disrupts normal learning and social behavior in rats, and these effects could be related to alterations of amygdala function. ECOTOXICITY STUDIES: A range of toxicity tests with aquatic organisms has indicated the adverse effects occur at exposure concentrations greater than 100 ug/L. Behavioral changes in fish were noted after sublethal BBP exposure.

Hazardous Substances Data Bank (HSDB)

12.1.2 NIOSH Toxicity Data





▶ The National Institute for Occupational Safety and Health (NIOSH)

12.1.3 Evidence for Carcinogenicity



CLASSIFICATION: C; possible human carcinogen. BASIS FOR CLASSIFICATION: Based on statistically significant increase in mononuclear cell leukemia in female rats; the response in male rats was inconclusive and there was no such response in mice. HUMAN CARCINOGENICITY DATA: None. ANIMAL CARCINOGENICITY DATA: Limited.

U.S. Environmental Protection Agency's Integrated Risk Information System (IRIS). Summary on Butyl benzyl phthalate (85-68-7). Available from, as of March 15, 2000: https://www.epa.gov/iris/

▶ Hazardous Substances Data Bank (HSDB)

Evaluation: There is inadequate evidence in humans for the carcinogenicity of butyl benzyl phthalate. There is limited evidence in experimental animals for the carcinogenicity of butyl benzyl phthalate. Overall evaluation: Butyl benzyl phthalate is not classifiable as to its carcinogenicity to humans (Group 3).

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: https://monographs.iarc.fr/ENG/Classification/index.php, p. 73 125

▶ Hazardous Substances Data Bank (HSDB)

12.1.4 Carcinogen Classification





IARC Carcinogenic Agent	Butyl benzyl phthalate		
IARC Carcinogenic Classes Group 3: Not classifiable as to its carcinogenicity to humans			
IARC Monographs	Volume Sup 7: Overall Evaluations of Carcinogenicity: An Updating of IARC Monographs Volumes 1 to 42, 1987; 440 pages; ISBN 92-832-1411-0 (out of print) Volume 73: (1999) Some Chemicals that Cause Tumours of the Kidney or Urinary Bladder in Rodents and Some Other Substances		

International Agency for Research on Cancer (IARC)

12.1.5 Exposure Routes



The substance can be absorbed into the body by inhalation of its aerosol and by ingestion.

▶ ILO International Chemical Safety Cards (ICSC)

12.1.6 Acute Effects



▶ ChemIDplus

12.1.7 Interactions



Although risk assessments are typically conducted on a chemical-by-chemical basis, the 1996 Food Quality Protection Act (FQPA) required the Environmental Protection Agency (EPA) to consider cumulative risk of chemicals that act via a common mechanism of toxicity. To this end, we are conducting studies with mixtures to provide a framework for assessing the cumulative effects of "antiandrogenic" chemicals. Rats were dosed during pregnancy with antiandrogens singly or in pairs at dosage levels equivalent to about one half of the ED50 for hypospadias or epididymal agenesis. The pairs include: AR antagonists (vinclozolin plus procymidone), phthalate esters (DBP plus BBP and DEHP plus DBP), a phthalate ester plus an AR antagonist (DBP plus procymidone), and linuron plus BBP. We predicted that each chemical by itself would induce few malformations; however, by mixing any two chemicals together, about 50% of the males would be malformed. All binary combinations produced cumulative, dose-additive effects on the androgens "inhibition of androgen synthesis". In this study, the complex mixture behaved in a dose-additive manner. Our results indicate that compounds that act by disparate mechanisms of toxicity display cumulative, dose-additive effects when present in combination. /Mixtures/

PMID:19147833

Rider CV et al; Toxicol Pathol. 37 (1): 100-13 (2009)

▶ Hazardous Substances Data Bank (HSDB)

Butyl benzyl phthalate (BBP), an endocrine disruptor present in the environment, exerts its genomic effects via intracellular steroid receptors and elicits non-genomic effects by interfering with membrane ion-channel receptors. We previously found that BBP blocks the calcium signaling coupled with P2X receptors in PC12 cells (Liu & Chen, 2006). Osteoblast P2X receptors were recently reported to play a role in cell proliferation and bone remodeling. In this present study, the effects of BBP on ATP-induced responses were investigated in human osteosarcoma HOS cells. These receptors mRNA had been detected, named P2X4, P2X7, P2Y2, P2Y4, P2Y5, P2Y9, and P2Y11, in human osteosarcoma HOS cells by RT-PCR. The enhancement of cell proliferation and the decrease of cytoviability had both been shown to be coupled to stimulation via different concentrations of ATP. BBP suppressed the ATP-induced calcium influx (mainly coupled with P2X) and cell proliferation but not the ATP-induced intracellular calcium release (mainly coupled with P2Y) and cytotoxicity in human osteosarcoma HOS cells. Suramin, a common P2 receptor's antagonist, blocked the ATP-induced calcium signaling, cell proliferation, and cytotoxicity. We suggest that P2X is mainly responsible for cell proliferation, and P2Y might be partially responsible for the observed cytotoxicity. BBP suppressed the calcium signaling coupled with P2X, suppressing cell proliferation. Since the importance of P2X receptors during bone metastasis has recently become apparent, the possible toxic risk of environmental BBP during bone remodeling is a public problem of concern.

PMID:20114058

Liu PS, Chen CY.; Toxicol Appl Pharmacol. 244 (3): 308-14 (2010)

▶ Hazardous Substances Data Bank (HSDB)

During recent decades the prevalence of IgE-mediated (atopic) allergic diseases in Western Europe and the USA has been increasing dramatically. It has been suggested that one possible cause is the presence in the environment of chemicals that may act as adjuvants, enhancing immune and allergic responses. Certain commonly used **phthalate** plasticizers such as butyl benzyl phthalate (BBP) have been implicated in this way. In the current experiments, the impact of BBP, applied by a physiologically relevant exposure route, on the vigour of immune responses induced in BALB/c strain mice has been examined. Mice were immunized via subcutaneous injection with the reference allergen ovalbumin (OVA) and received concurrent topical treatment with doses of BBP that induced significant changes in liver weight. The generation of specific anti-OVA IgE and IgG1 antibodies was measured by passive cutaneous anaphylaxis and by enzyme-linked immunosorbant assays, respectively. Topical administration of BBP was without impact on anti-OVA IgE antibody responses, regardless of whether BBP was applied locally or distant to the site of OVA immunization. However, same-site treatment with high-dose BBP (100 mg) did result in a modest elevation in anti-OVA IgG1 antibody production, a subclass of antibody used as a surrogate marker of IgE responses. Taken together with human exposure data, these results suggest that the doses of **phthalate** encountered in the home environment are unlikely to be a major factor contributing to the increased incidence of asthma and allergy in the developed world.

PMID:18816477

Dearman RJ et al; J Appl Toxicol. 29 (2): 118-25 (2009)

▶ Hazardous Substances Data Bank (HSDB)

12.1.8 Antidote and Emergency Treatment



Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Esters and related compounds/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 253

▶ Hazardous Substances Data Bank (HSDB)

Basic treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary. Monitor for shock and treat if necessary ... For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with 0.9% saline (NS) during transport ... Do not use emetics. For ingestion, rinse mouth and administer 5 mL/kg up to 200 mL of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal ... /Esters and related compounds/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 253

▶ Hazardous Substances Data Bank (HSDB)

Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in severe respiratory distress. Positive-pressure ventilation techniques with a bag-valve-mask device may be beneficial. Consider drug therapy for pulmonary edema Monitor cardiac rhythm and treat arrhythmias if necessary Start IV administration of D5W TKO /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's (LR) if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Consider vasopressors if patient is hypotensive with a normal fluid volume. Watch for signs of fluid overload Use proparacaine hydrochloride to assist eye irrigation ... /Esters and related compounds/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds.).; Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 254

▶ Hazardous Substances Data Bank (HSDB)

12.1.9 Medical Surveillance

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Liver and kidney function tests. Examination of the nervious system, including nerve conduction tests.

Sittig, M. Handbook of Toxic and Hazardous Chemicals and Carcinogens, 2002. 4th ed.Vol 1 A-H Norwich, NY: Noyes Publications, 2002., p. 406

Hazardous Substances Data Bank (HSDB)

12.1.10 Human Toxicity Excerpts



/HUMAN EXPOSURE STUDIES/ Exposure to phthalic acid esters, mainly di-(2-ethylhexyl), diisodecyl and butylbenzyl phthalates, or workers in a **polyvinyl chloride** processing industry ranged from 0.02 to 2 mg/cu m in different job categories. The workers excreted slightly but significantly higher levels of phthalic acid ester metabolites in urine than controls. In 54 workers studied clinically, there were no indications of peripheral nerve or respiratory system effects. Some biochemical tests were abnormal.

PMID:4072908

Nielson J et al; Am Ind Hyg Assoc J 46 (11): 643-7 (1985)

▶ Hazardous Substances Data Bank (HSDB)

/HUMAN EXPOSURE STUDIES/ Workers in a PVC processing plant, exposed to to diisodecyl phthalate and/or butylbenzyl phthalate in the air, showed statistically higher levels of phthalate acid ester (not specified) in urine than workers of the control group; contrary to earlier finding no clinically obvious cases of polyneuropathy were detected.

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program's Robust Summaries and Test Plans. Available from the Database Query page at: https://www.epa.gov/hpv/pubs/hpvrstp.htm on Phthalate Esters Category, Benzyl butyl phthalate (85-68-7) p. 32 (2007) as of April 28, 2008.

► Hazardous Substances Data Bank (HSDB)

/HUMAN EXPOSURE STUDIES/ In the general population, a significant increase in the risk of bronchial obstruction during the first 2 years of life has been related to presence of PVC flooring (adjusted O.R greater than or equal to 1.89) in a case control study of 251 children and an equal number of matched controls. ...

DHHS/NTP-CERHR Monograph on the Potential Human Reproductive and Developmental Effects of Butyl Benzyl Phthalate (BBP) p. 19 (2003) NIH Publication No. 03-4487

/EPIDEMIOLOGY STUDIES/ ... Dose-response associations of decreased semen quality with urinary concentrations of) and ... metabolites of dibutyl phthalate and butylbenzyl phthalate /were reported/ ... The present study /examines/ ... a larger sample of men and includes measurements of di(2-ethylhexyl) phthalate (DEHP) oxidative metabolites. ... Between January 2000 and May 2004, ... 463 male partners of subfertile couples who presented for semen analysis to the Massachusetts General Hospital /were recruited/. Semen parameters were dichotomized based on World Health Organization reference values for sperm concentration (<20 million/mL) and motility (<50% motile) and the Tygerberg Kruger Strict criteria for morphology (<4% normal). The comparison group was men with all 3 semen parameters above the reference values. In a single spot urine sample from each man, phthalate metabolites were measured using solid-phase extraction coupled to high-performance liquid chromatography isotope-dilution tandem mass spectrometry. RESULTS: There were dose-response relationships of monobutyl phthalate (MBP with low sperm concentration (odds ratio per quartile adjusted for age, abstinence time, and smoking status = 1.00, 3.1, 2.5, 3.3; P for trend = 0.04) and motility (1.0, 1.5, 1.5, 1.8; P for trend = 0.04). There was suggestive evidence of an association between the highest monobenzyl phthalate (MBzP) quartile and low sperm concentration (1.00, 1.1, 1.1, 1.9; P for trend = 0.13). There were no relationships of monoethyl phthalate, and the DEHP metabolites with these semen parameters. The present study confirms previous results on the relationship of altered semen quality with exposure to MBP at general population levels. /No associations between semen parameters and 3 DEHP metabolites were found./

Hauser R et al; Epidemiology 17 (6): 682-91 (2006)

▶ Hazardous Substances Data Bank (HSDB)

For more Human Toxicity Excerpts (Complete) data for BUTYL BENZYL PHTHALATE (22 total), please visit the HSDB record page.

▶ Hazardous Substances Data Bank (HSDB)

12.1.11 Non-Human Toxicity Excerpts



/LABORATORY ANIMALS: Acute Exposure/ ... /It was/ reported that 0.5 mL of neat BBP applied on the abraded or unabraded skin of rabbits for 24 hr produced essentially no irritation.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 873

▶ Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Acute Exposure/ Intradermal injections into rabbits produced no inflammatory response as indicated by dye extravasation after 10 min, there was a mild response after 15 min and moderate response after 26 min. /from table/

Casarett, L.J., and J. Doull. Toxicology: The Basic Science of Poisons. New York: MacMillan Publishing Co., 1975., p. 610

▶ Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ Like other **phthalate** diesters, butyl benzyl phthalate increases the weight of the liver in rats. When administered at dietary levels of 0.6, 1.2 or 2.5% for 21 days to male and female Fischer 344 rats, butyl benzyl phthalate produced hepatic peroxisome proliferation, with weak induction of peroxisomal activity (**palmitoyl-coenzyme A** oxidation) in both males and females. Microsomal activites (**lauric acid** 12-hydroxylase) were strongly induced in males but hardly at all in females. Ultrastructural examination of liver sections revealed an increase in the numbers of peroxisomes.

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: https://monographs.iarc.fr/ENG/Classification/index.php, p. V73 119 (1999)

▶ Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ Sprague-Dawley rats were administered BBP in the diet for 3 mo at dose levels of 0, 188, 375, 1125 or 1500 mg/kg/day (males) and 188, 375, 750, 1125, or 1500 mg/kg/day (females). No compound-related lesions were observed at necropsy or on histopathological examination. Relative liver weight was increased at 750 mg/kg/day and higher in females, and at 1125 mg/kg/day and higher in males. In male rats, relative kidney weight increased at 750 mg/kg/day and higher. A NOAEL of 375 mg/kg/day was established based on liver and kidney effects at 750 mg/kg/day.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 868

► Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Excerpts (Complete) data for BUTYL BENZYL PHTHALATE (89 total), please visit the HSDB record page.

12.1.12 Non-Human Toxicity Values





LD50 Rat oral 2330 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 401

▶ Hazardous Substances Data Bank (HSDB)

LD50 Rat Oral 2-20 g/kg /2,000-20,000 mg/kg/

DHHS/NTP-CERHR Monograph on the Potential Human Reproductive and Developmental Effects of Butyl Benzyl Phthalate (BBP) p. 19 (2003) NIH Publication No. 03-4487

▶ Hazardous Substances Data Bank (HSDB)

LD50 Rat dermal 6700 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 401

▶ Hazardous Substances Data Bank (HSDB)

LD50 Mouse oral 4170 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 401

▶ Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Values (Complete) data for BUTYL BENZYL PHTHALATE (10 total), please visit the HSDB record page.

▶ Hazardous Substances Data Bank (HSDB)

12.1.13 Ecotoxicity Values



EC50; Species: Selenastrum capricornutum (alga); Concentration: 110 ug/L for 96 hr; toxic effect: chlorophyll a /Conditions of bioassay not specified in source examined/ USEPA; Ambient Water Quality Criteria Doc: Phthalate Esters p.B-13 (1980) EPA 440/5-80-067

▶ Hazardous Substances Data Bank (HSDB)

EC50; Species: Selenastrum capricornutum (alga); Concentration: 130 ug/L for 96 hr; toxic effect: cell number /Conditions of bioassay not specified in source examined/ USEPA; Ambient Water Quality Criteria Doc: Phthalate Esters p.B-13 (1980) EPA 440/5-80-067

▶ Hazardous Substances Data Bank (HSDB)

EC50; Species: Skeletonema costatum (alga); Concentration: 170 ug/L for 96 hr; toxic effect: chlorophyll a /Conditions of bioassay not specified in source examined/

USEPA; Ambient Water Quality Criteria Doc: Phthalate Esters p.B-13 (1980) EPA 440/5-80-067

▶ Hazardous Substances Data Bank (HSDB)

EC50; Species: Skeletonema costatum (alga); Concentration: 190 ug/L for 96 hr; toxic effect: cell number /Conditions of bioassay not specified in source examined/ USEPA; Ambient Water Quality Criteria Doc: Phthalate Esters p.B-13 (1980) EPA 440/5-80-067

▶ Hazardous Substances Data Bank (HSDB)

For more Ecotoxicity Values (Complete) data for BUTYL BENZYL PHTHALATE (42 total), please visit the HSDB record page.

12.1.14 Ecotoxicity Excerpts





/BIRDS and MAMMALS/ ... The effect of endocrine disrupting chemicals (EDCs) ... on 3,3',5-L-(1251)triiodothyronine ((1251)T3) binding to purified Japanese quail transthyretin (gTTR), a major thyroid hormonebinding protein in plasma, and to the ligand-binding domain of thyroid hormone receptor beta (qTR LBD). Scatchard plots of T3 binding to qTTR and qTR LBD revealed two classes of binding sites, with Kd values of 6.9 and 185 nM, and a single class of binding sites, with Kd value of 0.31 nM, respectively. ... Although ... n-butylbenzyl phthalate /was an effective inhibitor of (1251)T3 binding to gTTR, its/ potency was two orders of magnitude less than that of T3. All test chemicals except for diethylstilbestrol had either a weak or no effect on (125I)T3 binding to qTR LBD...

PMID:13129501

Ishihara A et al: Gen Comp Endocrinol 134 (1): 36-43 (2003)

▶ Hazardous Substances Data Bank (HSDB)

/AQUATIC SPECIES/ The aguatic toxicity of phthalic acid, six monoesters, and five diesters of o-phthalic acid was tested in three standardized toxicity tests using the bacteria Vibrio fischeri, the green algae Pseudokirchneriella subcapitata, and the crustacean Daphnia magna. The monoesters tested were monomethyl, monobutyl, monobutyl, monobenzyl, mono(2-ethylhexyl), and monodecyl phthalate, while the diesters tested were dimethyl, diethyl, organisms ranged from 103 mg/L to >4,710 mg/L for phthalic acid, and corresponding values for the monoesters ranged from 2.3 mg/L (monodecyl phthalate in bacteria test) to 4,130 mg/L (monomethyl phthalate in bacteria test). Dimethyl and diethyl phthalate were found to be the least toxic of the diesters (EC50 26.2-377 mg/L), and the toxicity of the other diesters (butylbenzyl and dibutyl phthalate) ranged from 0.96 to 7.74 mg/L. In general, the phthalate monoesters (degradation products) were less toxic than the corresponding diesters (mother compounds).

Jonsson S, Baun A; Environ Toxicol Chem 22 (12): 3037-43 (2003)

▶ Hazardous Substances Data Bank (HSDB)

/AQUATIC SPECIES/ ...The 3,5,3'-L-triiodothyronine (T3)- uptake system on the plasma membrane of Rana catesbeiana tadpole red blood cells (RBCs) /was characterized in the presence of a variety of inhibitors ... RBCs were incubated with [125I]T3 in the presence of each chemical. Among the test chemicals, di-n-butyl phthalate /and/ n-butylbenzyl phthalate ... were the most powerful inhibitors of (125I)T3 uptake, with an IC50 of 2.2 uM, which was one order of magnitude greater than that for T3 (IC50, 0.14 uM) ...

PMID:15590988

Shimada N, Yamauchi K; J Endocrinol 183 (3): 627-37 (2004)

▶ Hazardous Substances Data Bank (HSDB)

/AQUATIC SPECIES/ ... Effects of sublethal concentrations of p,p'-2,2-bis(p-chlorophenyl)-1,1-dichloroethylene (DDE) and butylbenzylphthalate (BBP) on feeding behavior in threespine stickleback Gasterosteus aculeatus. The fish were exposed for 31 days to either BBP (10 or 100 ug/L) or DDE (5 or 50 ug/L) or to a mixture of BBP and DDE in the corresponding concentrations. Five weeks after exposure termination, ... fish that had been exposed to the higher concentrations of DDE and/or BBP initiated feeding more often than control fish. The latency time to feeding (ranging from 0.25 to 5.0 min) differed between control fish and fish exposed to mixtures of DDE and BBP. ...

PMID:14759668

Wibe AE et al; Ecotoxicol Environ Saf 57 (2): 213-9 (2004)

▶ Hazardous Substances Data Bank (HSDB)

For more Ecotoxicity Excerpts (Complete) data for BUTYL BENZYL PHTHALATE (18 total), please visit the HSDB record page.

▶ Hazardous Substances Data Bank (HSDB)

12.1.15 Ongoing Test Status



EPA has released the first beta version (version 0.5) of the Interactive Chemical Safety for Sustainability (iCSS) Dashboard. The beta version of the iCSS Dashboard provides an interactive tool to explore rapid, automated (or in vitro high-throughput) chemical screening data generated by the Toxicity Forecaster (ToxCast) project and the federal Toxicity Testing in the 21st century (Tox21) collaboration. /The title compound was tested by ToxCast and/or Tox21 assays; Click on the "Chemical Explorer" button on the tool bar to see the data./[USEPA; ICSS Dashboard Application; Available from, as of December 8, 2014: http://actor.epa.gov/dashboard/]

▶ Hazardous Substances Data Bank (HSDB)

The following link will take the user to the National Toxicology Program (NTP) Test Agent Search Results page, which tabulates all of the "Standard Toxicology & Carcinogenesis Studies", "Developmental Studies", and "Genetic Toxicity Studies" performed with this chemical. Clicking on the "Testing Status" link will take the user to the status (i.e., in review, in progress, in preparation, on test, completed, etc.) and results of all the studies that the NTP has done on this chemical. [Available from: http://ntp-apps.niehs.nih.gov/ntp_tox/index.cfm?fuseaction=ntpsearch.searchresults&searchterm=85-68-7]

▶ Hazardous Substances Data Bank (HSDB)

12.1.16 National Toxicology Program Studies





A carcinogenesis bioassay of butyl benzyl phthalate ... was accomplished by feeding diets containing 6,000 or 12,000 ppm of the **phthalate** to groups of 50 F344/N rats and 50 B6C3F1 mice of each sex for 28 to 103 wk. ... After wk 14, an increasing number of dosed male rats died as a result of an unexplained internal hemorrhaging, and all surviving male rats were /sacrificed/ at wk 29 to 30. Because of cmpd related mortality, butyl benzyl phthalate was not adequately tested for carcinogenicity in male F344/N rats. ... Under the conditions of this bioassay, butyl benzyl phthalate was probably carcinogenic for female F344/N rats, causing an incr incidence of mononuclear cell leukemias. The male F344/N rat study was considered inadequate for the evaluation due to cmpd related toxicity and early mortality. Butyl benzyl phthalate was not carcinogenic for B6C3FI mice of either sex. Levels of Evidence of Carcinogenicity: Male Rats: Inadequate Study; Female Rats: Positive; Male Mice: Negative; Female Mice: Negative.

Carcinogenesis Bioassay of Butyl Benzyl Phthalate in F344/N Rats and B6C3F1 mice (Feed Study) Technical Report Series No. 213 (1982) NIH Publication No. 82-1769 U.S. Department of Health and Human Services, National Toxicology Program, National Institute of Environmental Health Sciences, Research Triangle Park, NC 27709

▶ Hazardous Substances Data Bank (HSDB)

... Male and female F344/N rats were given butyl benzyl phthalate (at least 97% pure) in feed for ... 2 yr. ... 2 YEAR STUDY IN RATS: Groups of 60 male F344/N rats were given 0, 3,000, 6,000, or 12,000 ppm butyl benzyl phthalate (equivalent to average daily doses of approx 120, 240 or 500 mg butyl benzyl phthalate/kg body weight), and groups of 60 female F344/N rats were given 0, 6,000, 12,000 or 24,000 ppm butyl benzyl phthalate (equivalent to average daily doses of approx 300, 600 or 1,200 mg/kg) in feed for 2 yr. ... CONCLUSIONS: Under the conditions of this 2 yr feed study, there was some evidence of carcinogenic activity of butyl benzyl phthalate in male F344/N rats based on the increased incidences of pancreatic acinar cell adenoma and of transitional epithelial papilloma of the urinary bladder.

Toxicology & Carcinogenesis Studies of Butyl Benzyl Phthalate in F344/N Rats (Feed Studies). Technical Report Series No. 458 (1997) NIH Publication No. 97-3374 U.S. Department of Health and Human Services, National Toxicology Program, National Institute of Environmental Health Sciences, Research Triangle Park, NC 27709

▶ Hazardous Substances Data Bank (HSDB)

Butyl benzyl phthalate (BBP) ... was evaluated for maternal and developmental toxicity in timed- pregnant Swiss albino (CD-l) mice (n=28-30 per group, except n=14 at 2.0% butyl benzyl phthalate). Butyl benzyl phthalate (0, 0.1, 0.5, 1.25 or 2.0% in feed) was administered between the mornings of gestational day (gd) 6 and 15. At sacrifice (gestational day 17), the status of implantation sites was recorded; each fetus was weighed and examined for external, visceral and skeletal malformations. No maternal or embryo/fetal effects were observed at 0.1% butyl benzyl phthalate (0.182 g/kg/day). At 0.5% butyl benzyl phthalate (0.910 g/kg/day), maternal effects were limited to a 15% reduction in wt. gain during treatment. The percent nonlive implants/litter (i.e., resorptions plus late fetal deaths) was increased at 0.5% butyl benzyl phthalate (15% vs. 8% for controls), as was the percent fetuses malformed/litter (14% vs. 4%). Dams in the 1.25% butyl benzyl phthalate (2.330 g/kg/day) group showed a 71% reduction in gestational wt. gain, a 66% reduction in treatment wt. gain, and a 25% reduction in corrected wt. gain. Absolute liver wt. was decreased, and relative liver and kidney wts. were increased in the absence of treatment-related microscopic lesions. Relative food intake (g/kg/day) was increased by 27% (gestational days 15 to 17) and relative water intake by 35-36% (gestational days 12 to 17). Also at 1.25% butyl benzyl phthalate, the percent nonlive implants/litter was increased (93% vs. 8%), average fetal body wt./litter was reduced by 17%, and the percent malformed fetuses/litter was increased (89% vs. 4%). The 2.0% butyl benzyl phthalate dose (4.121 g/kg/day) was eliminated after evaluation of 14 dams since all implanted conceptuses were resorbed. In summary, 0.1% dietary butyl benzyl phthalate was a no-observed-adverse-effect level (NO AEL) for both maternal and developmental toxicity. At 0.5%, butyl benzyl phthalate and 2.0%, significant maternal and embryo/fetal effects were observed, including greater than

Department of Health & Human Services/National Institute of Environmental Health Sciences, National Toxicology Program; Developmental Toxicity of Butyl benzyl phthalate (CAS No. 85-68-7) in CD-1 Swiss Mice, NTP Study No. TER89026 (June 22,1990) Available from, as of August 15, 2002: https://ntp.niehs.nih.gov/index.cfm?objectid=0847FF31-90CC-C685-88B4D7EAC975BD44

▶ Hazardous Substances Data Bank (HSDB)

Butyl benzyl phthalate (BBP), a phthalate ester plasticizer, was evaluated for maternal and developmental toxicity in timed-pregnant Sprague-Dawley derived (CD) rats (27-30/group). Butyl benzyl phthalate (0, 0.5, 1.25 or 2.0%) in feed between the mornings of gestational day (gd) 6 and 15 yielded average doses of 0, 0.42, 1.10 or 1.64 g butyl benzyl phthalate/kg/day, respectively. At sacrifice (gestational day 20), the status of

implantation sites was recorded; each fetus was weighed and examined for external, visceral and skeletal malformations. No maternal or embryo/fetal effects were observed at 0.5% butyl benzyl phthalate other than increased relative water intake (g/kg/day) between gestational days 15 and 18. Dams in the 1.25% butyl benzyl phthalate group exhibited a 37% reduction in weight gain during treatment, increased relative liver wt., increased relative food intake (11-25% after gestational day 12), and increased relative water intake (18-41% after gestational day 9). At 1.25% butyl benzyl phthalate, the percent fetuses with variations/litter was increased, and the percent fetuses malformed/litter (5.9% vs. 2% for controls) approached statistical significance. Dams in the 2% butyl benzyl phthalate group showed a 93% reduction in treatment weight gain, and a 17% reduction in corrected weight gain. Relative liver and kidney weights were increased. Relative food intake was initially decreased (14% for gestational days 6 to 9), and later increased (16-44% after gd 12). Relative water intake was increased (25-73% after gd 9). At 2% butyl benzyl phthalate, the resorptions/litter were increased (40% vs. 4% for controls), average fetal body weight/litter was reduced by 20%, and the percent malformed fetuses/litter was increased (53% vs. 2% for controls). In summary, 0.5% dietary butyl benzyl phthalate was a no-observed-adverse-effect level (NO AEL) for both maternal and developmental toxicity. The mid-dose (1.25% butyl benzyl phthalate) produced significant maternal toxicity and minimal evidence of developmental toxicity. At the high dose (2% butyl benzyl phthalate), significant maternal and developmental toxicity was observed, including an increased incidence of malformations.

Department of Health & Human Services/National Institute of Environmental Health Sciences, National Toxicology Program; Developmental Toxicity of Butyl Benzyl Phthalate (CAS No. 85-68-7) Administered in Feed to CD Rats on Gestational Days 6 to 15, NTP Study No. TER88025 (August 4, 1989) Available from, as of August 15, 2002: https://ntp.niehs.nih.gov/index.cfm?objectid=0847FF31-90CC-C685-88B4D7EAC975BD44

▶ Hazardous Substances Data Bank (HSDB)

12.1.17 TSCA Test Submissions





Effects on the liver and liver lipids were evaluated in groups of male and female Fischer 344 rats (5/sex/dose level) fed nominal levels of 0, 1.2 or 2.5% butyl benzyl phthalate in the diet for 21 days. Toxicity was evident by statistical differences between dosed groups and controls for: mean body weights (2.5 and 1.2% group males & 2.5% group females), food consumption values (2.5% group males & females), relative liver and kidney weights (all treated groups) and relative testis weights (2.5% group males). There was a statistically significant decrease in serum triglyceride levels for the 1.2 and 2.5% group males and a significant increase in triglycerides for the 2.5% group females. There was a moderate increase in the amount of peroxisome proliferation for the high dose animals. Liver biochemistry revealed statistically significant differences between treated groups and controls as indicated by cyanide-insensitive palmitoyl-CoA oxidation levels (all treated males & 2.5% group females), lauric acid 11- and 12- hydroxylase activities (all treated males & 2.5% group females) and hepatic microsomal protein levels (2.5% group males). There was no consistent dose response relationship among the treatment groups for lipid content in the liver. Histological changes attributable to butyl benzyl phthalate were reduction in cytoplasmic basophilia in the livers of the high dose rats. Also at the 2.5% dietary level, butyl benzyl phthalate caused severe testicular atrophy.

The British Industrial Biological Research Association; A 21-Day Feeding Study of Butyl Benzyl Phthalate to Rats: Effects on the Liver and Liver lipids, (1985), EPA Document No. 40+8626201, Fiche No. OTS0509543

▶ Hazardous Substances Data Bank (HSDB)

The toxicity of butyl benzyl phthalate was evaluated in the mouse lymphoma L5178Y cell line in the presence and absence of rat liver S9 metabolic activation. All cultures were treated in duplicate with concentrations of 9.77, 19.50, 39.10, 78.10, 156.00, 313.00, 625.00, 1250.00, 2500.00 or 5000.00 nL/mL, and growth was determined at 24 and 48 hours after initiation of the treatment. Under nonactivated conditions, butyl benzyl phthalate was soluble up to 313 nL/mL, and treatments at 625 nL/mL and 1250 nL/mL were highly toxic (less than 2% of the relative suspension growth). Treatments at 2500 nL/mL were lethal to nonactivated cultures. Assays with metabolic activation were soluble up to 1250 nL/mL and produced moderate toxicity at 1250 nL/mL (average percent suspension growth, 25% of the solvent (acetone) control). Treatments at 2500 nL/mL and 5000 nL/mL were lethal to activated cultures.

Litton Bionetics; Evaluation of Butyl Benzyl Phthalate in the Mouse Lymphoma Toxicity Assay, Final Report, (1985), EPA Document No. 40+8526206, Fiche No.OTS0509537

▶ Hazardous Substances Data Bank (HSDB)

The ability of butyl benzyl phthalate to induce morphological transformation was evaluated in the Balb/c-3T3 A-31 mouse cell line (Cell Transformation Assay). Based on preliminary toxicity determinations (exposure time = 72 hr), butyl benzyl phthalate, was tested at concentrations of 10.0, 20.0, 40.0, 80.0 or 160.0 nL/mL, resulting in a range of 90% to 8% relative survival. None of the treatments produced significantly greater transformation frequencies (95% confidence level) relative to the negative control (culture medium).

Litton Bionetics; Evaluation of Butyl Benzyl Phthalate in the In-vitro Transformation of Balb/3T3 Cells Assay, Final Report), (1985), EPA Document No. 40+8526206, Fiche No. OTS0509537

Hazardous Substances Data Bank (HSDB)

The ability of butyl benzyl phthalate to induce specific locus mutations at the TK locus in cultured L5178Y mouse lymphoma cells (Mouse Lymphoma Mutagenicity Assay) was evaluated in the presence and absence of Aroclor-induced rat liver S-9 metabolic activation. Based on preliminary toxicity tests, 16 nonactivated cultures treated from 6.25 nL/mL to 40.0 nL/mL were cloned, producing a range of 83 - 2.5% relative growth. Twenty S-9 activated cultures treated from 200 to 1400 nL/mL were cloned, producing a range of 65.7 - 1.0% relative growth. None of the cultures produced mutant frequencies significantly greater than the solvent control (acetone).

Hazleton Biotechnologies Company; Mutagenicity of Butyl Benzyl Phthalate in a Mouse Lymphoma Mutation Assay, Final Report, (1986), EPA Document No. 40-8626225, Fiche No. OTS0510527

12.1.18 Populations at Special Risk





Phthalates are used widely in consumer products. Exposure to several phthalates has been associated with respiratory symptoms and decreased lung function. Associations between children's phthalate exposures and fractional exhaled nitric oxide (Fe(NO)), a biomarker of airway inflammation, have not been examined. We hypothesized that urinary concentrations of four phthalate metabolites would be positively associated with Fe(NO) and that these associations would be stronger among children with seroatopy or wheeze. In an urban ongoing birth cohort, 244 children had phthalate metabolites determined in urine collected on the same day as Fe(NO) measurement. Repeated sampling gathered 313 observations between ages 4.9 and 9.1 years. Seroatopy was assessed by specific IqE. Wheeze in the past year was assessed by validated questionnaire. Regression models used generalized estimating equations. Log-unit increases in urinary concentrations of metabolites of diethyl phthalate (DEP) and butylbenzyl phthalate (BBzP) were associated with a 6.6% (95% confidence interval [CI] 0.5-13.1%) and 8.7% (95% CI, 1.9-16.0%) increase in Fe(NO), respectively, adjusting for other phthalate metabolites and potential covariates/confounders. There was no association between concentrations of metabolites of di(2-ethylhexyl) phthalate or di-n-butyl phthalate and Fe(NO). There was no significant interaction by seroatopy. The BBzP metabolite association was significantly stronger among children who wheeze (P = 0.016). Independent associations between exposures to DEP and BBzP and Fe(NO) in a cohort of inner-city children were observed. These results suggest that these two ubiquitous phthalates, previously shown to have substantial contributions from inhalation, are positively associated with airway inflammation in children.

PMID:22923660

Soil

Full text: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3530221 Just AC et al; Am J Respir Crit Care Med. 186 (9): 830-7 (2012)

▶ Hazardous Substances Data Bank (HSDB)

12.2 Ecological Information

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12.2.1 US EPA Regional Screening Levels for Chemical Contaminants

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Resident Soil (mg/kg)	2.90e+02
Industrial Soil (mg/kg)	1.20e+03
Tapwater (ug/L)	1.60e+01
Risk-based SSL (mg/kg)	2.40e-01
Oral Slope Factor (mg/kg- day)-1	1.90e-03
Chronic Oral Reference Dose (mg/kg-day)	2.00e-01
Fraction of Contaminant Absorbed in Gastrointestinal Tract	1
Fraction of Contaminant Absorbed Dermally from	0.1

▶ US EPA Regional Screening Levels for Chemical Contaminants at Superfund Sites

12.2.2 US EPA Regional Removal Management Levels for Chemical Contaminants



Resident Soil (mg/kg)	2.90e+04
Industrial Soil (mg/kg)	1.20e+05
Tapwater (ug/L)	1.60e+03
Oral Slope Factor (mg/kg- day)-1	1.90e-03

Chronic Oral Reference Dose (mg/kg-day)	2.00e-01
Fraction of Contaminant Absorbed in Gastrointestinal Tract	1
Fraction of Contaminant Absorbed Dermally from Soil	0.1

▶ US EPA Regional Screening Levels for Chemical Contaminants at Superfund Sites

12.2.3 ICSC Environmental Data

The substance is very toxic to aquatic organisms. Bioaccumulation of this chemical may occur in fish.

▶ ILO International Chemical Safety Cards (ICSC)

12.2.4 Environmental Fate/Exposure Summary



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Butyl benzyl phthalate's production and use as a plasticizer for polyvinyl and cellulose resins, as an organic intermediate and in the production of vinyl tiles may result in its release to the environment through various waste streams. The US Congress has permanently banned benzyl butyl phthalate in any amount greater than 0.1 percent in children's toys and certain child care articles. If released to air, a vapor pressure of 8.25X10-6 mm Hg at 25 °C indicates butyl benzyl phthalate will exist in both the vapor and particulate phases in the atmosphere. Vapor-phase butyl benzyl phthalate will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 35 hours. Particulate-phase butyl benzyl phthalate will be removed from the atmosphere by wet and dry deposition. Butyl benzyl phthalate contains chromophores that absorb at wavelengths > 290 nm and, therefore, may be susceptible to direct photolysis by sunlight. If released to soil, butyl benzyl phthalate is expected to have low to no mobility based upon log Koc values of 3.21-3.997. Volatilization from moist soil surfaces is expected based upon an estimated Henry's Law constant of 1.3X10-6 atm-cu m/mole. However, adsorption to soil is expected to attenuate volatilization. Butyl benzyl phthalate is not expected to volatilize from dry soil surfaces based upon its vapor pressure. Utilizing the Japanese MITI test, 80.9% of the theoretical BOD was reached in 2 weeks indicating that biodegradation is an important environmental fate process. If released into water, butyl benzyl phthalate is expected to adsorb to suspended solids and sediment based upon the log Koc value of >4.7 measured in suspended solids. Biodegradation in river die-away tests resulted in half-lives of approximately 0.32 to 13 days, suggesting that biodegradation is an important environmental fate process in water. Volatilization from water surfaces is expected based upon this compound's estimated Henry's Law constant. Estimated volatilization half-lives for a model river and model lake are 52 and 380 days, respectively. However, volatilization from water surfaces is expected to be attenuated by adsorption to suspended solids and sediment in the water column. The volatilization halflife from a model pond is about 380 years when adsorption is considered. A BCF of 9.4 reported in bluegill sunfish suggests bioconcentration in aquatic organisms is low. Hydrolysis is not expected to be an important process except under basic conditions based on estimated hydrolysis half-lives of 1.4 years and 51 days at pHs 7 and 8, respectively. Occupational exposure to butyl benzyl phthalate may occur through inhalation of aerosols and dermal contact with this compound at workplaces where butyl benzyl phthalate is produced or used. Monitoring data indicate that the general population may be exposed to butyl benzyl phthalate via inhalation of ambient air, ingestion of food and drinking water, and dermal contact with consumer products containing butyl benzyl phthalate. (SRC)

▶ Hazardous Substances Data Bank (HSDB)

12.2.5 Artificial Pollution Sources



Butyl benzyl phthalate's production and use as a plasticizer for polyvinyl and cellulose resins, as an organic intermediate(1) and in the production of vinyl tiles(2) may result in its release to the environment through various waste streams(SRC). Effective January 1, 2012, the US Congress has permanently banned three types of phthalates (di-(2-ethylhexyl) phthalate (DEHP), dibutyl phthalate (DBP), or benzyl butyl phthalate) in any amount greater than 0.1 percent (computed for each phthalate, individually) in children's toys and certain child care articles. The ban applies to products manufactured after December 31, 2011 - Consumer Product Safety Improvement Act of 2008 (CPSIA)(3).

(1) Lewis RJ Sr; Hawley's Condensed Chemical Dictionary, 15th ed. New York, NY; Van Nostrand Reinhold Co., p. 196 (2007) (2) National Toxicology Program. Center for the Evaluation of Risks to Human Reproduction. Monograph on the Potential Human Reproductive and Developmental Effects of Butyl Benzyl Phthalate (BBP). Available from, as of March 18, 2015: https://ntp.niehs.nih.gov/ntp/ohat/phthalates/bb-phthalate/bbp_monograph_final.pdf (3) US CPSC; Phthalates. Washington, DC: US Consumer Products Safety Comm. Available from, as of March 11, 2015: https://www.cpsc.gov/en/Business--Manufacturing/Business-Education/Business-Guidance/Phthalates-Information/

12.2.6 Environmental Fate



TERRESTRIAL FATE: Based on a classification scheme(1), log Koc values of 3.21-3.997(2-4), indicate that butyl benzyl phthalate is expected to have low to no mobility in soil(SRC). Volatilization of butyl benzyl phthalate from moist soil surfaces is expected(SRC) given an estimated Henry's Law constant of 1.3X10-6 atm-cu m/mole(SRC), based upon its vapor pressure, 8.25X10-6 mm Hg(5), and water solubility, 2.69 mg/L(5). However, adsorption to soil is expected to attenuate volatilization(SRC). Butyl benzyl phthalate is not expected to volatilize from dry soil surfaces(SRC) based upon its vapor pressure(5). An 80.9% of theoretical BOD using activated sludge in the Japanese MITI test(6) suggests that biodegradation is an important environmental fate process in soil(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Zurmuehl T et al; J Contam Hydrol 8: 111-33 (1991) (3) Sabljic A et al; Chemosphere 31: 4489-514 (1995) (4) Thomsen M et al; Chemosphere 38: 2613-24 (1999) (5) Howard PH et al; Environ Toxicol Chem 4: 653-61 (1985) (6) NITE; Chemical Risk Information Platform (CHRIP). Biodegradation and Bioconcentration. Tokyo, Japan: Natl Inst Tech Eval. Available from, as of March 18, 2015: https://www.safe.nite.go.jp/english/db.html

▶ Hazardous Substances Data Bank (HSDB)

AQUATIC FATE: Based on a classification scheme(1), log Koc values of >4.7, measured in suspended solids(2), indicate that butyl benzyl phthalate is expected to adsorb to suspended solids and sediment(SRC). Volatilization from water surfaces is expected(3) based upon an estimated Henry's Law constant of 1.3X10-6 atm-cu m/mole(SRC), derived from its vapor pressure, 8.25X10-6 mm Hg(4), and water solubility, 2.69 mg/L(4). Using this Henry's Law constant and an estimation method(3), volatilization half-lives for a model river and model lake are 52 and 380 days, respectively(SRC). However, volatilization from water surfaces is expected to be attenuated by adsorption to suspended solids and sediment in the water column. The volatilization half-life from a model pond is about 380 years when adsorption is considered(5). The hydrolysis half-life of butyl benzyl phthalate was calculated to be 1.4 years and 51 days at pH values of 7 and 8, respectively(6). According to a classification scheme(7), a BCF of 9.4 in bluegill sunfish(8), suggests bioconcentration in aquatic organisms is low(SRC). Biodegradation in river die-away tests resulted in half-lives of approximately 0.32(9) to 13 days(10), suggesting that biodegradation may be an important environmental fate process in water(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Ritsema R et al; Chemosphere 18: 2161-75 (1989) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 7-4, 7-5, 15-1 to 15-29 (1990) (4) Howard PH et al; Environ Toxicol Chem 4: 653-61(1985) (5) US EPA; EXAMS II Computer Simulation (1987) (6) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov. 2012. Available from, as of March 18, 2015: https://www.epa.gov/oppt/exposure/pubs/episuitedl.htm (7) Franke C et al; Chemosphere 29: 1501-14 (1994) (8) Carr KH et al; Environ Toxicol Chem 16: 2200-3 (1997) (9) Peterson DR, Staples; Handbook of Environ Chem 3: 85-124 (2003) (10) Carson DB et al; pp. 48-59 in Aquatic Toxicol Risk Assess 13: ASTM STP 1096 (1990)

▶ Hazardous Substances Data Bank (HSDB)

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), butyl benzyl phthalate, which has a vapor pressure of 8.25X10-6 mm Hg at 25 °C(2), will exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase butyl benzyl phthalate is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals(SRC); the half-life for this reaction in air is estimated to be 35 hours(SRC), calculated from its rate constant of 1.1X10-11 cu cm/molecule-sec at 25 °C(SRC) that was derived using a structure estimation method(3).

Particulate-phase butyl benzyl phthalate may be removed from the air by wet and dry deposition(SRC). Butyl benzyl phthalate contains chromophores that absorb at wavelengths >290 nm(4) and, therefore, may be susceptible to direct photolysis by sunlight(SRC).

(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) Howard PH et al; Environ Toxicol Chem 4: 653-61 (1985) (3) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of March 18, 2015: https://www.epa.gov/oppt/exposure/pubs/episuitedl.htm (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 8-12 (1990)

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12.2.7 Environmental Biodegradation





AEROBIC: Butyl benzyl phthalate was degraded 74-79% in 10-50 days at 25 °C from an initial concentration of 100 mg/L, using 30 mg/L activated sludge(1). Butyl benzyl phthalate was completely biodegraded in Rhine River water over a 6 day incubation period(2). Butyl benzyl phthalate incubated in a lake water/sediment microcosm biodegraded to intermediates with a half-life of 5 days and was completely biodegraded with a half-life of about 13 days, when incubated in river water a half-life of 2 days was reported for the degradation to intermediates(3). Butyl benzyl phthalate was biodegraded 93 and >99% using a semi-continuous activated sludge with starting concentrations of 3.3 and 133.3 mg/L, respectively(4). Butyl benzyl phthalate had half-lives of 1.5 and 0.32 days in river die-away tests with a starting concentration of 1 mg/L and 1 ug/L, and a half-life of 1.4 days using a lake microcosm(5). Butyl benzyl phthalate, at a concentration of 20 ppm, digested for 28 days had 87% degradation(6). Using a fresh water inoculum, butyl benzyl phthalate was degraded 100% in 7 days from a starting concentration of 1 ppm(6). Butyl benzyl phthalate, present at 100 mg/L, reached 80.9% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test(7).

(1) Desai SM; Diss Abstr Int B 52: 3752 (1992) (2) Ritsema R et al; Chemosphere 18: 2161-75 (1989) (3) Carson DB et al; in Aquatic Toxicol Risk Assess 13: ASTM STP 1096 pp. 48-59 (1990) (4) Saeger VW, Tucker ES; Appl Environ Microbiol 31: 29-34 (1976) (5) Peterson DR, Staples; Handbook of Environ Chem 3: 85-124 (2003) (6) Staples CA et al; Chemosphere 35: 667-749 (1997) (7) NITE; Chemical Risk Information Platform (CHRIP). Biodegradation and Bioconcentration. Tokyo, Japan: Natl Inst Tech Eval. Available from, as of March 18, 2015: https://www.safe.nite.go.jp/english/db.html

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AEROBIC: Using sewage sludge from a waste water treatment plant in Taoyaun, Taiwan, aerobic biodegradation rate constants under varying pH and temperature were analyzed for butyl benzyl phthalate(1):

рН	Temp (deg C)	Rate (k/day)	Half-life (days)
3	30	0.136	5.1
5	30	0.210	3.3
7	30	0.332	2.1
9	30	0.231	3.0
11	30	0.131	5.3
7	20	0.245	2.8
7	30	0.193	3.6
7	40	0.169	4.1
7	55	0.141	4.9

(1) Chang BV et al; Chemosphere 69: 1116-23 (2007)

▶ Hazardous Substances Data Bank (HSDB)

ANAEROBIC: The half-life of butyl benzyl phthalate in an anaerobic sewage sludge was measured as 107 hours(1). Butyl benzyl phthalate had a 91% methane production after 35-100 days from a starting concentration of 20 ug/L(2). Butyl benzyl phthalate was biodegraded anaerobically 98.3% after a 120 day digestion at 35 °C(3). Butyl benzyl phthalate had half-lives of 12.4 and 7.2 days from a starting concentration of 20 mg/L in sludge and 40% diluted sludge, respectively(4). Butyl benzyl phthalate, incubated at 35 °C for 56 days, was biodegraded 24% from a starting concentration of 68 ppm(5). With a starting concentration of 20 ppm, incubated at 35 °C for 70 days, butyl benzyl phthalate was biodegraded 100%(5). The biodegradation of butyl benzyl phthalate in samples inoculated with fresh water sediment, salt marsh sediment and digester sludge was 12, 3 and 50% in 35, 36 and 29 days, respectively: digestions were done at 35 °C under anaerobic conditions(6).

(1) Ziogou K et al; Water Res 23: 743-48 (1989) (2) Ejlertsson J et al; Environ Sci Technol 31: 2761-4 (1997) (3) Parker WJ et al; Water Res 28: 1779-89 (1994) (4) Peterson DR, Staples CA; Handbook of Environ Chem 3: 85-124 (2003) (5) Staples CA et al; Chemosphere 35: 667-749 (1997) (6) Painter SE, Jones WJ; Environ Technol 11: 1015-26 (1990)

▶ Hazardous Substances Data Bank (HSDB)

12.2.8 Environmental Abiotic Degradation



The rate constant for the vapor-phase reaction of butyl benzyl phthalate with photochemically-produced hydroxyl radicals has been estimated as 1.1X10-11 cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 35 hours at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(1). A base-catalyzed second-order hydrolysis rate constant of 0.16 L/mole-sec(SRC) was estimated using a structure estimation method(1); this corresponds to half-lives of 1.4 years and 51 days at pH values of 7 and 8, respectively(1). Butyl benzyl phthalate contains chromophores that absorb at wavelengths >290 nm(2) and, therefore, may be susceptible to direct photolysis by sunlight(SRC).

(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of March 18, 2015: https://www.epa.gov/oppt/exposure/pubs/episuitedl.htm (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 8-12, 8-13 (1990)

▶ Hazardous Substances Data Bank (HSDB)

12.2.9 Environmental Bioconcentration



Bioconcentration Factor

16.22

▶ EPA DSSTox

Bluegill sunfish (Lepomis macrochirus) exposed to 9.73 ug/L of C14 labeled butyl benzyl phthalate for 21 days had a measured BCF values of 663 and 772(1). However, these studies used total radioactive residues in whole fish to calculate the BCF; the metabolism of butyl benzyl phthalate in the fish was not considered(1). Bluegill sunfish exposed to uniformly ring labeled butyl benzyl phthalate for 3.27 days had a BCF of 9.4(1). According to a classification scheme(2), BCF values of zero to 30 are low and from 100 to 1,000 are high. Biota-sediment accumulation factors for butyl benzyl phthalate were 4.3, 4.6 and 2.8 in roach (Rutilus

rutilus), chub (Leuciscus cephalus) and perch (Perca fluviatilis), respectively; fish were collected from the Orge River, France from Jul 2009 to Apr 2010(3). BCFs of 0.13-45 were reported for butyl benzyl phthalate in water spinach (Ipomoea aquatica) grown under different conditions on sludge from waste water treatment plants in China(4).

(1) Carr KH et al; Environ Toxicol Chem 16: 2200-3 (1997) (2) Franke C et al; Chemosphere 29: 1501-14 (1994) (3) Teil M et al; Arch Environ Contam Toxicol 63: 101-13 (2012) (4) Cai QY et al; Bull Environ Contam Toxicol 77: 411-8 (2006)

Hazardous Substances Data Bank (HSDB)

12.2.10 Soil Adsorption/Mobility



Soil Adsorption Coefficient

5.25e+03 L/kg

▶ EPA DSSTox

A log Koc value of 3.3 was measured from unsaturated soil columns at pH 4.8(1). Other experimental log Koc values given are 3.21(2) and 3.997(3). According to a classification scheme(4), these Koc values suggest that butyl benzyl phthalate is expected to have low to no mobility in soil. An experimental log Koc of >4.7 was determined from sediment samples from Lake Yssel, the Netherlands(5).

(1) Zurmuehl T et al; J Contam Hydrol 8: 111-33 (1991) (2) Sabljic A et al; Chemosphere 31: 4489-514 (1995) (3) Thomsen M et al; Chemosphere 38: 2613-24 (1999) (4) Swann RL et al; Res Rev 85: 23 (1983) (5) Ritsema R et al; Chemosphere 18: 2161-75 (1989)

▶ Hazardous Substances Data Bank (HSDB)

12.2.11 Volatilization from Water/Soil



The Henry's Law constant for butyl benzyl phthalate is estimated as 1.3X10-6 atm-cu m/mole(SRC) derived from its vapor pressure, 8.25X10-6 mm Hg(1), and water solubility, 2.69 mg/L(1). This Henry's Law constant indicates that butyl benzyl phthalate is expected to volatilize from water surfaces(2). Based on this Henry's Law constant, the volatilization half-life from a model river (1 m deep, flowing 1 m/sec, wind velocity of 3 m/sec)(2) is estimated as 52 days(SRC). The volatilization half-life from a model lake (1 m deep, flowing 0.05 m/sec, wind velocity of 0.5 m/sec)(2) is estimated as 380 days(SRC). However, volatilization from water surfaces is expected to be attenuated by adsorption to suspended solids and sediment in the water column. The volatilization half-life from a model pond is about 380 years when adsorption is considered(3). Butyl benzyl phthalate's Henry's Law constant indicates that volatilization from moist soil surfaces may occur(SRC). Butyl benzyl phthalate is not expected to volatilize from dry soil surfaces(SRC) based upon its vapor pressure(1).

(1) Howard PH et al; Environ Toxicol Chem 4: 653-61 (1985) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990) (3) US EPA; EXAMS II Computer Simulation (1987)

▶ Hazardous Substances Data Bank (HSDB)

12.2.12 Environmental Water Concentrations





GROUNDWATER: Butyl benzyl phthalate was identified, not quantified, in groundwater near a landfill in Oklahoma(1), and at a maximum concentration of 2 ug/L in groundwater near a chemical plant in Michigan(2). Butyl benzyl phthalate was detected in the Biscayne Aquifer groundwater at a maximum of 20 ug/L and was not detected in well fields(3). A sand and gravel aquifer in Pensacola, FL had butyl benzyl phthalate concentrations of 91 ug/L at the Cypress Street location in samples taken July 28, 1981(4). Butyl benzyl phthalate was not detected (detection limit 0.18 ng/L) in a ground water sample collected in Catalonia, Spain in Nov 2007(5).

(1) Sawhney BL; in Reactions and Movements of Organic Chemicals in Soils, SSSA Special Publication 22 pp. 447-74 (1989) (2) USEPA; Superfund Record of Decision (EPA Region 5): Ott/Story/Cordova Chemical Site, North, Muskegon, Michigan (First Remedial Action), September 1989. Washington, DC: USEPA, Off Emerg Rem Response. USEPA/EOD/R05-89/111 (NTIS PB90-138405) pp. 103 (1989) (3) Canter LW, Sabatini DA; Int J Environ Stud 46: 35-57 (1994) (4) Troutman DE et al; US Geological Survey. Water-Resources Investigations Report 84-4230 pp. 40 (1984) (5) Sanchez-Avila J et al; Sci Total Environ 407: 4157-67 (2009)

▶ Hazardous Substances Data Bank (HSDB)

DRINKING WATER: Butyl benzyl phthalate was identified, not quantified, in Cincinnati, OH drinking water(1). The maximum reported concentrations of butyl benzyl phthalate reported in drinking water were 0.1 ppb in Philadelphia(1), and 1.8 ug/L in New Orleans(2). Butyl benzyl phthalate was detected at a maximum of 20 ug/L in a survey of 49 drinking water sites in the US(3). Butyl benzyl phthalate was detected in 5 out of 39 public water system wells in New York State; the highest concentration found was 38 ppb(4). Butyl benzyl phthalate was detected at a maximum of 38 ppb in a survey of US drinking water facilities(5). Butyl benzyl phthalate was detected in 2 of 19 source water samples at 53 and 54 ng/L, but not detected (detection limit 50 ng/L) in finish or tap water samples from these 19 water utilities located throughout the US;

samples were collected 2006 and 2007(6). Butyl benzyl phthalate was detected in 5 of 15 finished drinking water samples from four water filtration plants in San Diego County, CA at 0.056-0.911 ug/L, sample dates were Aug 2001 to Jun 2002(7).

(1) Kopfler FC et al; Amer Chem Soc Natl Mtg Div Env Chem Prep 15: 185-7 (1975) (2) Keith LH et al; pp. 329-73 in Identification and analysis of organic pollutants in water. Keith LH ed., Ann Arbor, MI: Ann Arbor Press (1976) (3) Canter LW, Sabatini DA; Int J Environ Stud 46: 35-57 (1994) (4) Kim NK, Stone DW; Organic chemicals and drinking water. Albany, NY: New York State Dept of Health (1980) (5) Steelman BL, Ecker RM; Organics Contamination of Groundwater: An Open Literature Review. Richland, WA: Battele Pacific Northwest Lab, DE-AC06-76RLO (1984) (6) Benotti MJ et al; Environ Sci Technol 43: 597-603 (2009) (7) Loraine GA, Pettigrove ME; Environ Sci Technol 40: 687-95 (2006)

▶ Hazardous Substances Data Bank (HSDB)

SURFACE WATER: Butyl benzyl phthalate was found in the Delaware River at 0.6 ppb(1) and at 2.4 ug/L in Mississippi River near St. Louis(2). Butyl benzyl phthalate was identified, not quantified, in Lake Michigan water(3). Butyl benzyl phthalate was detected at 15 ng/L and 200 ng/L in the aqueous and particulate form, respectively, from 357 samples taken from the St. Lawrence River, sampled 1981 to 1987(4). Butyl benzyl phthalate, analyzed in the Potomac River, Quantico, VA in 1986 was found at <2 ug/L(5). Butyl benzyl phthalate was detected in 16 of 16 and 14 of 15, samples collected from Eleven Points and the north fork of White River, MO, at 0.8-144 and 0.8-351 ng/L, respectively; samples were collected Aug 2003 to Nov 2004(6). Butyl benzyl phthalate was detected in the Rhine River in the Netherlands at <1 ug/L(7) and 0.022-0.060 ug/L(8). Butyl benzyl phthalate was detected in the Mersey Estuary in the UK at 0-0.135 ug/L(9). Butyl benzyl phthalate was found in 22% of 116 samples taken from rivers, lakes and channels in 1997 in Germany at an average of 2.95 ug/L(10). Butyl benzyl phthalate was detected in Huaihe River, China in the summer of 2002 at 0.69-1.24, 0.61-1.08, and 0.83-1.59 ug/L at Xiao Zui, Huaihe River bridge, and Hongguang Chemical plant, respectively(11). Butyl benzyl phthalate was not detected in 43 surface water samples collected through out Korea in 2002(12).

(1) Hites RA; pp. 107-20 in Natl Conf Munic Sludge Manage 8th (1979) (2) Gledhill WE et al; Env Sci Tech 14: 301-5 (1980) (3) Konasewich D et al; Status report on organic and heavy metal contaminants in the Lakes Erie, Michigan, Huron and Superior Basins; Great Lake Water Qual Board (1978) (4) Germain A, Langlois C; Water Pollut Res J Can 23: 602-14 (1988) (5) Hall LW Jr et al; Aquat Toxicol 10: 73-99 (1987) (6) Solis ME et al; Arch Environ Contam Toxicol 53: 426-34 (2007) (7) Ritsema R et al; Chemosphere 18: 2161-75 (1989) (8) Hendricks AJ et al; Water Res 28: 591-98 (1994) (9) Preston MR, Al-Omran LA; Environ Pollut 62: 183-93 (1989) (10) Fromme H et al; Water Res 36: 1429-38 (2002) (11) Huang H et al; Bull Environ Contam Toxicol 73: 339-46 (2004) (12) Yoon J et al; Organohalogen Compounds 66: 1436-40 (2004)

▶ Hazardous Substances Data Bank (HSDB)

RAIN/SNOW: Snow surface analysis were done in the Antarctic in 1993/1994 season, results for butyl benzyl phthalate in subsurface snow samples at McCarthy Ridge were 23 ng/L at 1 meter deep, 15 ng/L at 2 meters deep and 52 ng/L at 3 meters deep(1). Butyl benzyl phthalate subsurface snow samples taken at Hercules Neve were all below detection limit at 1, 2 and 3 meters deep(1). Butyl benzyl phthalate was identified in 6 of 10 snow sample sites; 0.82 ug/kg at Nellim (Lapland, Finland), 0.87 ug/kg at Muonio (Lapland, Finland), 0.81 ug/kg at Levi (Lapland, Finland), 0.07 ug/kg at Butovo (Moscow, Russia), 3.05 ug/kg at Shosse (Entuziastov, Russia), and 0.17 ug/kg at Baikal'sk (Lake Baikal, Siberia)(2).

(1) Desideri PG et al; Int J Environ Anal Chem 71: 331-51 (1998) (2) Poliakova OV et al; Toxicol Environ Chem 75: 181-94 (2000)

Hazardous Substances Data Bank (HSDB)

SEAWATER: Butyl benzyl phthalate was detected at 1.89-6.41 ng/L in samples collected from 4 locations in False Creek Harbor, Vancouver, Canada; freely dissolved concentrations in the same samples were 0.97-3.28 ng/g; sampling dates were not reported(1). Butyl benzyl phthalate was detected in 5, 8 and 3 seawater samples from the Norwegian Coast, lower and central Arctic at 6-48, 1-7 and <0.2-2 pg/L, respectively; samples were collected from a ship Jul 17 to Aug 28, 2004(2).

(1) MacKintosh CE et al; Environ Sci Technol 40: 3481-8 (2006) (2) Xie Z et al; Environ Sci Technol 41: 4555-60 (2007)

▶ Hazardous Substances Data Bank (HSDB)

12.2.13 Effluent Concentrations



Butyl benzyl phthalate was found at a maximum concentration of 2000 ug/kg from soil, sediment and waste piles from Bayou Bonfouca remediation area, Slidell, LA(1). Butyl benzyl phthalate is commonly found in landfill leachate in the US at concentrations of 5.1-8.0 ug/L(2). Butyl benzyl phthalate was found in 30, 40, 70, and 100% of sediment samples taken near combined sewer overflow in the lower Passaic River in NJ at Worthington Avenue, Second River Union, Herbert Place, and Ivy Street, respectively(3). Hazardous waste incinerators in the US released 114 tons of butyl benzyl phthalate in 1990(4). Butyl benzyl phthalate was detected in the ashes of 8 municipal refuse incinerator sampled in 1987 from around the US at not detected to 1200 ug/kg(5). Butyl benzyl phthalate was detected in sediment of a waste disposal facility in Kansas at 11,000 ug/kg(6). For samples collected from 1981 to 1986, butyl benzyl phthalate was detected in 5.7%, 1.3%, 1.0%, 0.8%, 2.7%, 7.1%, 3.0% and 2.2% of the hazardous waste site groundwater samples in EPA regions 1, 2, 4, 5, 6, 8, 9 and 10, respectively(7). Butyl benzyl phthalate was not detected in regions 3 and 7(7). Butyl benzyl phthalate was detected in 1 of 102 effluent samples from 52 treatment facilities located throughout Oregon at 1030 ng/L; samples were collected the summer and fall of 2010(8).

(1) Acharya P, Ives P; J Air Waste Manage Assoc 44: 1195-1203 (1994) (2) Christensen TH et al; Crit Rev Environ Sci Technol 24: 194-202 (1994) (3) Iannuzzi TJ et al; Chemosphere 17: 21-34 (1997) (4) Dempsey CR; J Air Waste Manage Assoc 43: 1374-79 (1993) (5) Shane BS et al; Arch Environ contam Toxicol 19: 665-73 (1990) (6) USEPA; Superfund Record of Decision (EPA Region 7): Doepke Disposal (Holliday), KS. (First Remedial Action), September 1989. Washington, DC: USEPA, Off Emerg Rem Response. USEPA/ROD/R07-89/032 (NTIS PB90-162645) pp. 84 (1989) (7) Plumb RH Jr; Environ Sci Pollut Control Ser 4: 173-197 (1992) (8) Hope BK et al; Sci Total Environ 417-418: 263-72 (2012)

Effluent from waste incinerators in West Germany contained butyl benzyl phthalate at 2.8 ug/cu m(1), 19.09 ng/cu m(2) and 17.46 ng/cu m(2). Butyl benzyl phthalate was detected in the leachate of a landfill in Sweden at concentrations of <5 to 8.1 ug/L(3). Butyl benzyl was found at 0.04-344.1 mg/kg dry weight from household waste leachates(4). Butyl benzyl phthalate was not detected in 4 domestic sewages, 6 domestic sewages with storm runoff and small industrial effluent, or 2 domestic sewages with storm runoff and large industrial effluent(5). Butyl benzyl phthalate was found in 54 of 275 samples at 10.1-82.9 ug/L with positive samples from 14 of 37 municipal water pollution control plants tested(6). Butyl benzyl phthalate was not found in 3 waste water effluents from a petrochemical plant, was not found in industrial landfill leachate sampled Dec 1996 but, was found at 3.0 ug/L in the industrial landfill leachate sampled March 1997(7). Butyl benzyl phthalate was found in 18% of 34 samples taken from sewage treatment plant effluent in 1997 in Germany at an average concentration of 0.7 ug/L and was not detected in sewage sludge, dump runoff, compost water or liquid manure(8). Butyl benzyl phthalate was tested for in tire leachate water but not detected at a detection limit of 1.0 ug/L(9). Butyl benzyl phthalate was detected at 0.03-10.0 ug/L at 9 of 13 sampling points, representing domestic, industrial and mixed sewage input into the Mataro's waste water treatment plant, Catalonia, Spain, culminating to an influent concentration of 0.67 ug/L; effluent concentration was 0.01 ug/L; samples were collected Nov 21 and 28, 2007(10).

(1) Jay H, Stieglitz L; Chemosphere 30: 1249-60 (1995) (2) Wienecke J et al; Chemosphere 30: 907-13 (1995) (3) Oman C, Hynning PA; Environ Pollut 80: 265-71 (1993) (4) Bauer MJ, Herrmann R; Sci Total Environ 208:49-57 (1997) (5) Berset JD, Etter-Holzer R; J AOAC Int 84: 383-91 (2001) (6) Canviro Consultants; Ontario Ministry of the Environment Water Resources Branch. ISBN 0-7729-4900-X pp. 97 (1988) (7) Castillo M et al; Environ Sci Technol 32: 2180-4 (1998) (8) Fromme H et al; Water Res 36: 1429-38 (2002) (9) Nelson SM et al; Bull Environ Contam Toxicol 52: 574-81 (1994) (10) Sanchez-Avila J et al; Sci Total Environ 407: 4157-67 (2009)

Hazardous Substances Data Bank (HSDB)

12.2.14 Sediment/Soil Concentrations





SEDIMENT: Butyl benzyl phthalate was found in 16.9% of 429 sites sampled from 19 major US river basins from Aug 1992 to March 1995 with a maximum concentration of 2200 ug/kg (1). Butyl benzyl phthalate was detected in 5.6% of 536 sites samples Aug 1992 to Sept 1995 in 20 major river basins across the US with a maximum concentration of 2240 ug/kg dry weight(2). Butyl benzyl phthalate was identified, not quantified, in sediment from Newark Bay, NJ(3). Average butyl benzyl phthalate sediment concentrations in the Kanauha River, Lake Erie, the Mississippi River (Memphis) and the Missouri River were 0.13, 0.41, 0.63 and 0.23 ug/g, respectively(4). Butyl benzyl phthalate was found in 3 of 31 sediment samples taken from the Detroit River in 1982 at 0.12-0.22 mg/kg(5). Butyl benzyl phthalate was detected at 0-0.57 ug/kg in sediment samples from 38 stations collected June 1988 to April 1989 on the Calcasieu Estuary, LA(6). Butyl benzyl phthalate was found in surface sediment samples at 4 sites in False Creek in Vancouver, Canada(7). Samples taken in the summer of 1997 in Hamilton Harbour, Ontario had concentrations of butyl benzyl phthalate below the detection limit of 0.3 ug/g(8). Butyl benzyl phthalate was detected at 20.7-50.5 and 1250-5650 ng/g in sediment and suspended solids samples, respectively, collected from 4 locations in False Creek Harbor, Vancouver, Canada(9).

(1) Lopes TJ et al; pp 105-19 in Environ Toxicol Risk Assess: V7 ASTM STP 1333, Little EE et al, eds, Amer Soc Testing Materials (1997) (2) Lopes TJ, Furlong ET, Environ Sci Technol 20: 727-37 (2001) (3) Crawford DW et al; Ecotoxicol Environ Safety 30: 85-100 (1995) (4) Michael PR et al; Env Tox Chem 3: 377-89 (1984) (5) Great Lakes Water Quality Board; Report on the Great Lakes Water Quality. Great Lakes Surveillance, Vol 2 (1989) (6) Redmond MS et al; Arch Environ Contam Toxicol 30: 53-61 (1996) (7) Lin ZP et al; Environ Sci Technol 37: 2100-8 (2003) (8) McDowell DC, Metcalfe CD; J Great Lakes Res 27: 3-9 (2001) (9) MacKintosh CE et al; Environ Sci Technol 40: 3481-8 (2006)

▶ Hazardous Substances Data Bank (HSDB)

SOIL: Butyl benzyl phthalate was detected in soil at a gravel pit near Utica, NY at a concentration of 940 ug/kg(1). Soils from 10 Canadian agricultural areas were analyzed for butyl benzyl phthalate; it was not detected in one sample and nine samples tested below the method detection limit of 0.2 mg/kg dry weight(2). Butyl benzyl phthalate was detected in 30 soil samples from Beijing, China at not detected to 0.060 mg/kg dry weight(3). Soil samples collected from 26 sites in the JiangHan plain, China contained butyl benzyl phthalate at not detected to 81.9 ng/g in 46.2% of the samples; samples were collected June 2007 and Jan 2008(4).

(1) USEPA; Superfund Record of Decision (EPA Region 2): Ludlow Sand and Gravel Site, Town of Paris, Oneida County, New York (First Remedial Action), September 1988. Washington, DC: USEPA, Off Emerg Rem Response. USEPA/ROD/R02-88/067 (NTIS PB89-182521) pp. 78 (1989) (2) Webber MD, Wang C; Can J Soil Sci 75: 513-24 (1995) (3) Li XH et al; Bull Environ Contam Toxicol 77: 252-9 (2006) (4) Liu H et al; Chemosphere 78: 382-8 (2010)

▶ Hazardous Substances Data Bank (HSDB)

12.2.15 Atmospheric Concentrations



URBAN/SUBURBAN: Butyl benzyl phthalate was measured in 89 outdoor atmospheric samples with a range of 1-20 ng/cu m taken in the US, at a range of 0.38-1.78 ng/cu m in Canada, and at a range of <1-<10 ng/cu m in 32 samples taken in Europe(1), locations not specified. Butyl benzyl phthalate was detected in 10 of 10 urban traffic and 9 of 10 industrial sites from Thessaloniki, Greece at 0.04-0.98 and 0.11-0.80 ng/cu m, respectively; samples were collected Jan and Feb 2007(2). In samples taken May 2002 to Apr 2003 in Paris, France, butyl benzyl phthalate was detected at 0.5-12.2 ng/cu m in the vapor phase and 0.1-0.5 ng/cu m in the particulate form, respectively(3). Butyl benzyl phthalate was detected in urban and suburban air samples from Nanjing, China at 1.0-7.1 and 0.01-2.1 ug/cu m in the gas phase, and 0.15-1.7 and 0.02-0.7 ug/cu m in the particulate phase, respectively; samples were collected Apr, July, Oct 2005 and Jan 2006(4). Butyl benzyl phthalate was detected in all 33 air samples collected through out Korea in 2002 at 3-12 ug/cu m(5).

(1) Clark K et al; Handbook Environ Chem 3: 125-77 (2003) (2) Salapasidou M et al; Atmos Environ 45: 3720-9 (2011) (3) Teil MJ et al; Sci Total Environ 354: 212-23 (2006) (4) Wang P et al; Chemosphere 72: 1567-72 (2008) (5) Yoon J et al; Organohalogen Compounds 66: 1436-40 (2004)

INDOOR: Butyl benzyl phthalate was measured in 6 residential homes in Tokyo; concentrations were <0.0012-0.10 ug/cu m(1). Butyl benzyl phthalate was detected in indoor air at 20 ng/cu m(2). Butyl benzyl phthalate was detected at a maximum of 140 ng/cu m in 250 indoor samples taken in the US, and at <3-465 ng/cu m in 26 indoor samples taken in Europe(3).

(1) Otake T et al; Environ Sci Technol 35: 3099-102 (2001) (2) Weschler CJ; Environ Sci Technol 18: 648-52 (1984) (3) Clark K et al; Handbook Environ Chem 3: 125-77 (2003)

Hazardous Substances Data Bank (HSDB)

RURAL/REMOTE: Butyl benzyl phthalate was identified, not quantified, in the atmosphere of a forest in Germany(1). Butyl benzyl phthalate was detected in the gas and particulate form at 0.2-68 and 0.2-56 pg/cu m, respectively, in samples from over the ocean from the Norwegian coast to the Arctic sea; samples were collected Jul 17 to Aug 28, 2004(2).

(1) Helmig D et al; Atmos Environ 24A: 179-84 (1990) (2) Xie Z et al; Environ Sci Technol 41: 4555-60 (2007)

▶ Hazardous Substances Data Bank (HSDB)

SOURCE DOMINATED: Butyl benzyl phthalate was not detected in the atmosphere at flaming and smoldering stages of prescribed burning of two pine dominated forest areas of Georgia; fires were set in Apr 2004(1).

(1) Lee S et al; Environ Sci Technol 39: 9049-56 (2005)

▶ Hazardous Substances Data Bank (HSDB)

12.2.16 Food Survey Values





Butyl benzyl phthalate was analyzed for, but not detected in vodka(1). The mean butyl benzyl phthalate concentration was reported as 0.039, 0.4, 0.08, 7.4, 0.01, 0.13, 0.04, 0.005 and 0.09 ug/g in beverages, other dairy, eggs, fat and oils, fish, meat, poultry, vegetables and other foods, respectively(2). Food samples collected over four days from University P&M restaurant contained butyl benzyl phthalate at 63.0, 92.3, 3.27, 3.29 and 2.37 ng/g wet weight in lasagne, roast beef, fried vegetables, stewed apples and fruit salad, respectively(3). Butyl benzyl phthalate was not detected (detection limit 2 ng/g wet weight) in fish terrine, mixed salad, corn salad, radishes, chicken leg, mixed steak, Basmati rice, fried potatoes, plain yogurt, Gruyere cheese, Camembert cheese, granny apple or black grapes(3).

(1) Leibowitz JN et al; J AOAC Inter 78: 730-5 (1995) (2) Clark K et al; Handbook Environ Chem 3: 125-77 (2003) (3) Martine B et al; Bull Environ Contam Toxicol. 90(1): 91-6 (2013)

Hazardous Substances Data Bank (HSDB)

12.2.17 Plant Concentrations





Butyl benzyl phthalate was identified, not quantified, in plants and vegetation near a coal reclamation site in Illinois(1). Butyl benzyl phthalate was found in aquatic organisms June to Sept 1999 from False Harbor, Vancouver, British Columbia; green algae (Enteromorpha intestinalis; gutweed(2)) 2.56 ng/g lipid and brown algae (Nereocysitis luetkeana, Bull kelp(3), Fucus gardneri, Rockweed(3)) 2.29 ng/g lipid(4). Butyl benzyl phthalate was detected at 0.25-3.33 mg/kg dry weight in water spinach (Ipomoea aquatica) grown under different conditions on sludge from waste water treatment plants in China(5).

(1) Webber MD et al; J Environ Qual 23: 1019-26 (1994) (2) NaGISA; Grasskelp, Gutweed. National Geography In Shore Areas Project. Available from, as of May 20, 2015: https://nagisa.cbm.usb.ve/cms/shore-dwellers/grass-kelp-gutweed/(3) Washington State Univ; Beach Watchers. Intertidal Organisms EZ-ID Guides. Nereocystis luetkeana. Available from, as of May 20, 2015: https://www.beachwatchers.wsu.edu/ezidweb/seaweeds/ (4) MacKintosh CE et al; Environ Sci Technol 38: 2011-20 (2004) (5) Cai QY et al; Bull Environ Contam Toxicol 77: 411-8 (2006)

▶ Hazardous Substances Data Bank (HSDB)

Raw vegetables collected from 9 farms located in the Pearl River Delta area of Southern China contained butyl benzyl phthalate at the following concentrations(1):

nam vegetables concered from a farms focated in the real favor betta area of southern clima contained backy benzy, plantalate at the following concernations (1).			
Genus species	Common name	No. samples	Concn (mg/kg dry weight)
Brassica parachinensis	flowering Chinese cabbage	9	not detected-9.7
Brassica chinensis	paitsai	6	not detected-6.1
Ipomoea aquatica	spinach	8	not detected-8.10
Brassica juncea	mustard	5	0.59-0.63
Loctuca satira	lettuce	6	not detected-7.0
Vigna sesquipedalis	asparagus bean	3	not detected-1.2

Genus species	Common name	No. samples	Concn (mg/kg dry weight)
Amaranthus tricolor	edible amaranth	4	0.029-6.6
Momordica charantia	balsampear	1	not detected
Allium ascalonicum	shallot	1	2.4
Allium tuberosum	Chinese chive	1	0.79
Cucumis sativus	cucumber	1	not detected

⁽¹⁾ Mo CH et al; Arch Environ Contam Toxicol 56: 181-9 (2009)

12.2.18 Fish/Seafood Concentrations



Butyl benzyl phthalate was analyzed for but not found in edible fish from Wisconsin lakes and rivers(1). Three seaperch (Embiotoea lateralis) taken from False Creek, Vancouver, Canada contained 0.1 to 10 ppb of butyl benzyl phthalate (2). Butyl benzyl phthalate was found at 710 ug/kg in sea lamprey tissue collected from Brodhead Creek, Stroudsburg, PA on April 21, 1989(3).

(1) Devault DS; Arch Environ Contam Toxicol 14: 587-94 (1985) (2) Lin ZP et al; Environ Sci Technol 37: 2100-8 (2003) (3) Stephanatos BN, Knorr DF; Hydrocarbon Contam Soils 2: 811-28 (1992)

▶ Hazardous Substances Data Bank (HSDB)

Aquatic organisms collected June to Sept 1999 from False Harbor, Vancouver, British Columbia, Canada were analyzed for concentrations of butyl benzyl phthalate(1).

Organism	Genus species	Concn (ng/g lipid)
Blue mussels	Mytilus edulis	2.29
Pacific oysters	Crassostrea gigas	2.11
Geoduck clams	Panope abrupta	2.61
Manila clams	Tapes philippinarum	2.26
Dungeness crabs	Cancer magister	2.04
Purple seastar	Pisaster ochraccus	1.47
juvenile Shiner perch	Cyrnatogaster aggragata	1.93
Pacific herring	Clupea harengus pallasi	1.67
Pile perch	Thacochilus vacca	2.82
Striped seaperch	Embiotoca lateralis	2.90
Pacific staghorn sculpin	Leptocottus armatus	2.85
English sole	Pleuronectes ventulus	2.51
White-spotted greenling	Hexogrammos stelleri	2.15
Spiny dogfish	Squalus acanthias	muscle 1.61; liver 1.18; embryo 1.81
Surf scoters (bird)	Melanitta perspicillata	3.15
Plankton	phytoplankton, zooplankton, other pelagic invertebrates	2.83

⁽¹⁾ MacKintosh CE et al; Environ Sci Technol 38: 2011-20 (2004)



[▶] Hazardous Substances Data Bank (HSDB)

[▶] Hazardous Substances Data Bank (HSDB)

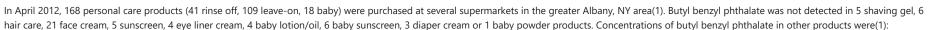
ENVIRONMENTAL: The mean concentration of butyl benzyl phthalate in dairy milk and infant formula powder was 0.0012 and 0.044 ug/g, respectively(1).

(1) Clark K et al; Handbook Environ Chem 3: 125-77 (2003)

▶ Hazardous Substances Data Bank (HSDB)

12.2.20 Other Environmental Concentrations





Product	Number	Mean (ug/g wet weight)	Maximum (ug/g wet weight)
Wash-off product			
Body wash	11	0.01	0.13
Shampoo	9	0.03	0.18
Hair conditioner	7	0.02	0.14
Face cleaner	9	0.01	0.10
Leave-on product			
Skin lotion	23	0.03	0.56
Perfume	12	6.70	78.3
Skin toner	9	0.01	0.06
Deodorant	14	0.01	0.14
Hand cream	3	0.03	0.09
Lipstick	4	0.05	0.70
Nail polish	8	0.70	2.20
Baby products			
Shampoo	4	0.04	0.14

(1) Guo Y, Kannan K; Environ Sci Technol; 47: 14442-9 (2013)

▶ Hazardous Substances Data Bank (HSDB)

Storm water runoff from roofs, parking area, vehicle service area, landscaped areas, urban creeks and detention ponds had butyl benzyl phthalate concentrations of 100, 12, 26, 130, 59 and 13 ug/L, respectively, in Alabama(1). Butyl benzyl phthalate was measured in personal air samples of pregnant New York women at 0.01-0.63 ug/cu m in samples taken Mar to Sept 2000 and in pregnant Krakow, Poland women at 0.00-0.19 ug/cu m in samples taken Nov 2000 to Mar 2001(2). Butyl benzyl phthalate was found at a median concentration of 31 mg/kg in 286 house dust samples(3). Butyl benzyl phthalate was detected in 6 of 6 residential and office dust samples at concentrations of 1.01-3.58 ug/g dust(4). Butyl benzyl phthalate was detected in 272 of 346 settled dust samples collected in children's bedrooms at 0.000-45.549 mg/g dust; samples were taken Oct 2001 to Apr 2002 from homes in Sweden(5). Butyl benzyl phthalate was detected in pillow protector, car interior cleaner and shaving cream samples at >1-100 ug/g; 213 commercial products representing 50 product types were analyzed(6).

(1) Pitt R et al; Water Environ Res 67: 260-75 (1995) (2) Adibi JJ et al; Environ Health Perspec 11: 1719-22 (2003) (3) Butte W, Heinzow B; Rev Environ Contam Toxicol 175: 1-46 (2002) (4) Rudel RA et al; J Air Waste Manage Assoc 51: 499-513 (2001) (5) Bornehag C-G et al; Environ Health Perspect 113: 1399-404 (2005) (6) Dodson RE et al; Environ Health Perspec 120: 935-43 (2012)

▶ Hazardous Substances Data Bank (HSDB)

Butyl benzyl phthalate was analyzed in house dust samples from six cities in China and one city in the US; samples were collected May to July 2010 and Dec 2007 to Jan 2008, respectively(1).

City	No. samples	Median concn (ug/g dw)	Range (ng/g dw)
Beijing	11	0.6	0.1-1.1

City	No. samples	Median concn (ug/g dw)	Range (ng/g dw)
Guangzhou	11	0.2	0.1-12.0
Jinan	13	0.1	not detected-0.1
Qiqihaer	12	0.2	0.2-0.6
Shanghai	21	0.2	not detected-7.4
Urumchi	7	0.4	0.2-1.2
Albany, NY	33	21.1	3.6-393

(1) Guo Y, Kannan K; Environ Sci Technol 45(8): 3788-94 (2011)

Hazardous Substances Data Bank (HSDB)

12.2.21 Probable Routes of Human Exposure





According to the 2012 TSCA Inventory Update Reporting data, 4 reporting facilities estimate the number of persons reasonably likely to be exposed in the manufacturing, processing, or use of butyl benzyl phthalate in the United States may be as low as <10 workers up to the range of 25-49 workers per plant; the data may be greatly underestimated due to confidential business information (CBI) or unknown values(1).

(1) US EPA; Chemical Data Reporting (CDR). Non-confidential 2012 Chemical Data Reporting information on chemical production and use in the United States. Available from, as of March 18, 2015: https://www.epa.gov/cdr/pubs/guidance/cdr_factsheets.html

▶ Hazardous Substances Data Bank (HSDB)

NIOSH (NOES Survey 1981-1983) has statistically estimated that 331,841 workers (59,743 of these are female) were potentially exposed to butyl benzyl phthalate in the US(1). Occupational exposure to butyl benzyl phthalate may occur through inhalation of aerosols and dermal contact with this compound at workplaces where butyl benzyl phthalate is produced or used. Monitoring data indicate that the general population may be exposed to butyl benzyl phthalate via inhalation of ambient air, ingestion of food and drinking water, and dermal contact with consumer products containing butyl benzyl phthalate(SRC).

(1) NIOSH; NOES. National Occupational Exposure Survey conducted from 1981-1983. Estimated numbers of employees potentially exposed to specific agents by 2-digit standard industrial classification (SIC). Available from, as of March 18, 2015: https://www.cdc.gov/noes/

▶ Hazardous Substances Data Bank (HSDB)

12.2.22 Average Daily Intake





The average daily intake of butyl benzyl phthalate was estimated as 0.085 ug/kg/day based on a food survey conducted in Albany, NY in 2011(1). The median concentration of monobenzyl phthalate in urine samples from 36 Japanese people collected May to June 2004 was 2.4 ug/L; this translates to an exposure rate of 0.074-0.11 ug/kg/day of the parent compound butyl benzyl phthalate(2). Based on analysis of urine samples from the German population, the average daily intake of butyl benzyl phthalate was 0.2-9.2, 0.2-6.8 and 0.2-4.5 ug/kg body weight/day in children, females and males, respectively(3).

(1) Schecter A et al; Environ Health Perspect 121: 473-9 (2013) (2) Itoh H et al; Environ Sci Technol 41: 4542-7 (2007) (3) Wormuth M et al; Risk Anal 26: 803-24 (2006)

▶ Hazardous Substances Data Bank (HSDB)

12.2.23 Body Burden



The mean concentration of butyl benzyl phthalate detected in human adipose tissue in the US was reported as 0.19 ug/g(1). Butyl benzyl phthalate was found in the serum of 2 of 41 young (17-47 months) Puerto Rican girls with premature breast development at 54-117 ug/L(2). The degradation product of butyl benzyl phthalate, monobenzyl phthalate (MBzP), was detected at 13.0-88.7 ug/g creatinine in 97% of 2540 urine samples collected in the United States National Health and Nutrition Examination Survey (1999-2000)(3). MbzP was detected in all 25 samples collected from pregnant New York women at 5.60-120 ug/g creatinine; samples were collected Mar to Sept 2000(4). MBzP was detected in >90% of the urine samples collected from 3236 people (ages 6-49 years old) during the Canadian Health Measures Survey 2007-2009(5). MBzP was detected in the serum of 350 of 501 female and 338 of 502 male seniors from Uppsala, Sweden at 0.38-17.3 and 0.41-35.7 mg/mL, respectively(6).

(1) USEPA; NHATS Broad Scan Analysis: Population Estiamtes from Fiscal Year 1982 Specimens. Washington, DC: USEPA, Off Tox Sub. USEPA 560/5-90-001 (1989) (2) Colon I et al; Environ Health Perspect 108: 895-900 (2000) (3) Silva MJ et al; Environ Health Perspect 112: 331-8 (2004) (4) Adibi JJ et al; Environ Health Perspect 11: 1719-22 (2003) (5) Saravanabhavan G et al; Int J Hyg Environ Health 216: 652-61 (2013) (6) Olsen L et al; Environ Saf 75: 242-8 (2012)

The butyl benzyl phthalate degradation product, **monobenzyl phthalate (MBzP)**, was analyzed in urine, breast milk and cord blood to determine exposure(1). Urine samples from 100 pregnant women were collected in the third trimester (Dec 2001-Nov 2002) and **MBzP** was detected in 64% of the samples at 0.08-235 ug/g. Urine samples from 30 two to three year olds (2003-2004) contained **MBzP** in 96% of the samples at 0.45-78.13 ug/g. Urine samples from 59 five to six year olds (2006-2007) contained **MBzP** in 97% of the samples at 0.35-79.10 ug/g. **MBzP** was detected in 3 of 30 cord blood samples that were collected upon delivery at <0.25-0.70 ug/L. All samples were collected from residents of central Taiwan(1).

(1) Lin S et al; Chemosphere 82: 947-55 (2011)

13 Associated Disorders and Diseases



▶ Comparative Toxicogenomics Database (CTD)

14 Literature

14.1 NLM Curated PubMed Citations

PubChem

14.2 Springer Nature References

Springer Nature

14.3 Depositor Provided PubMed Citations

② Z

PubChem

14.4 Chemical Co-Occurrences in Literature





PubChem

14.5 Chemical-Gene Co-Occurrences in Literature



PubChem

14.6 Chemical-Disease Co-Occurrences in Literature



PubChem

15 Patents

15.1 Depositor-Supplied Patent Identifiers



PubChem

Link to all deposited patent identifiers

PubChem

15.2 WIPO PATENTSCOPE

? Z

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=IRIAEXORFWYRCZ-UHFFFAOYSA-N

▶ PATENTSCOPE (WIPO)

16 Biomolecular Interactions and Pathways	
16.1 Protein Bound 3D Structures	② □

RCSB Protein Data Bank (RCSB PDB)

View 1 protein in NCBI Structure

PubChem

16.1.1 Ligands from Protein Bound 3D Structures		② <u>亿</u>
PDBe Ligand Code	27G	
PDBe Structure Code	4MG6	
PDBe Conformer		
▶ Protein Data Bank in	Europe (PDBe)	
16.2 Chemical-Gene Interactions		② Z
16.2.1 CTD Chemical	l-Gene Interactions	② 🗹

▶ Comparative Toxicogenomics Database (CTD)

17 Biological Test Results

17.1 BioAssay Results

② ☑

17.1 BioAssay Results

PubChem

18 Classification	② Z
18.1 Ontologies	② Z
18.1.1 MeSH Tree	② ☑

▶ Medical Subject Headings (MeSH)

18.1.2 ChEBI Ontology

② Z

▶ ChEBI





▶ KEGG

18.1.4 WHO ATC Classification System



▶ WHO Anatomical Therapeutic Chemical (ATC) Classification







▶ ChemIDplus

18.1.6 CAMEO Chemicals

CAMEO Chemicals

18.1.7 UN GHS Classification

▶ UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

18.1.8 EPA CPDat Classification



▶ EPA Chemical and Products Database (CPDat)

18.1.9 NORMAN Suspect List Exchange Classification





NORMAN Suspect List Exchange

18.1.10 EPA DSSTox Classification

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▶ EPA DSSTox

18.1.11 International Agency for Research on Cancer (IARC) Classification



▶ International Agency for Research on Cancer (IARC)



▶ Consumer Product Information Database (CPID)

19 Information Sources





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https://cameochemicals.noaa.gov/chemical/8354

CAMEO Chemical Reactivity Classification

https://cameochemicals.noaa.gov/browse/react

2. CAS Common Chemistry

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https://commonchemistry.cas.org/detail?cas_rn=85-68-7

3. ChemIDplus

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https://chem.nlm.nih.gov/chemidplus/sid/0000085687

ChemIDplus Chemical Information Classification

https://chem.nlm.nih.gov/chemidplus/

4. DTP/NCI

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https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=71001

5. EPA Chemicals under the TSCA

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1,2-Benzenedicarboxylic acid, 1-butyl 2-(phenylmethyl) ester https://www.epa.gov/chemicals-under-tsca

6. EPA DSSTox

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https://comptox.epa.gov/dashboard/DTXSID3020205

CompTox Chemicals Dashboard Chemical Lists

https://comptox.epa.gov/dashboard/chemical_lists/

7. European Chemicals Agency (ECHA)

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https://echa.europa.eu/web/guest/legal-notice

Benzyl butyl phthalate

https://echa.europa.eu/substance-information/-/substanceinfo/100.001.475

Benzyl butyl phthalate

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/103808

Benzyl butyl phthalate (BBP)

https://www.echa.europa.eu/substances-restricted-under-reach

Benzyl butyl phthalate (BBP)

https://www.echa.europa.eu/candidate-list-table

8. Hazardous Substances Data Bank (HSDB)

BUTYL BENZYL PHTHALATE

https://pubchem.ncbi.nlm.nih.gov/source/hsdb/2107

9. ILO International Chemical Safety Cards (ICSC)

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BUTYL BENZYL PHTHALATE

https://www.ilo.org/dyn/icsc/showcard.display?p_version=2&p_card_id=0834

10. NJDOH RTK Hazardous Substance List

butyl benzyl phthalate

http://nj.gov/health/eoh/rtkweb/documents/fs/2896.pdf

11. ChEBI

Butylbenzyl phthalate

http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:34595

ChEBI Ontology

http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology

12. Comparative Toxicogenomics Database (CTD)

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http://ctdbase.org/detail.go?type=chem&acc=C027561

13. Consumer Product Information Database (CPID)

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https://www.whatsinproducts.com/contents/view/1/6

Butyl benzyl phthalate

https://www.whatsinproducts.com/chemicals/view/1/486/000085-68-7

Consumer Products Category Classification

https://www.whatsinproducts.com/

14. EPA Chemical and Products Database (CPDat)

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https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

85-68-7

https://comptox.epa.gov/dashboard/DTXSID3020205#exposure

EPA CPDat Classification

https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat

15. EU REGULATION (EC) No 1272/2008

BBP; benzyl butyl phthalate

https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A32008R1272

16. Hazardous Chemical Information System (HCIS), Safe Work Australia

RRP

http://hcis.safeworkaustralia.gov.au/HazardousChemical/Details?chemicalID=343

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Butyl benzyl phthalate [BBP] - FY2016

https://www.nite.go.jp/chem/english/ghs/16-mhlw-0128e.html

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n-Butyl benzyl phthalate - FY2006

https://www.nite.go.jp/chem/english/ghs/06-imcg-0467e.html

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https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/

20. International Agency for Research on Cancer (IARC)

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https://monographs.iarc.who.int/list-of-classifications

IARC Classification

https://www.iarc.fr/

21. MassBank of North America (MoNA)

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http://mona.fiehnlab.ucdavis.edu/spectra/browse?inchikey=IRIAEXORFWYRCZ-UHFFFAOYSA-N

22. NIST Mass Spectrometry Data Center

Benzyl butyl phthalate http://www.nist.gov/srd/nist1a.cfm

23. Protein Data Bank in Europe (PDBe)

http://www.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/27G

24. RCSB Protein Data Bank (RCSB PDB)

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https://www.rcsb.org/

25. SpectraBase

Butyl benzyl phthalate

https://spectrabase.com/spectrum/F4cI6n9nSkE

Benzyl butyl phthalate

https://spectrabase.com/spectrum/E2Tl5qGtAev

PALATINOL BB

https://spectrabase.com/spectrum/FyyhjfEs5w5

BUTYL BENZYL PHTHALATE

https://spectrabase.com/spectrum/Jv9aqM9UMDX

SANTICIZER 160

https://spectrabase.com/spectrum/D8cTpiy8dAn

PALATINOL BB

https://spectrabase.com/spectrum/JERu1erBrtD

PHTHALIC ACID, BENZYL BUTYL ESTER

https://spectrabase.com/spectrum/lgVzwewaDmy

UNIMOLL B

https://spectrabase.com/spectrum/4LXzwQ6kEdO

benzylbutylphthalate

https://spectrabase.com/spectrum/8uacFXx9iEs

benzylbutylphthalate

https://spectrabase.com/spectrum/A7snzOtVZWO

butylbenzylphthalate

https://spectrabase.com/spectrum/o69P8nBFLT

PHTHALIC ACID, BENZYL BUTYL ESTER

https://spectrabase.com/spectrum/6A0Y4OUyZ1k

Phthalic acid, benzyl butyl ester

https://spectrabase.com/spectrum/39yavHda2un

phthalic acid, benzyl butyl ester

https://spectrabase.com/spectrum/C3G9oC9TYJa

PHTHALIC ACID. BENZYL BUTYL ESTER

https://spectrabase.com/spectrum/JfPujGkEmDq

Benzyl butyl phthalate

https://spectrabase.com/spectrum/HmcOcGn3F0A

1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester

https://spectrabase.com/spectrum/3U3NLCt92zs

1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester https://spectrabase.com/spectrum/EqJBYOAxWBx

BUTYLBENZYL PHTALATE

https://spectrabase.com/spectrum/AbaDVcuOahp

PHTHALIC ACID, (BENZYL)(BUTYL)ESTER

https://spectrabase.com/spectrum/Jfs5Y2TdKlK

1,2-BENZENEDICARBOXYLIC ACID, BUTYL PHENYLMETHYL ESTER

https://spectrabase.com/spectrum/46qWLv6exKa

Benzyl-butylphthalate

https://spectrabase.com/spectrum/IV8pcK43kMi

Benzyl-butylphthalate

https://spectrabase.com/spectrum/9YZpAjviFRA

Butylbenzylphthalate

https://spectrabase.com/spectrum/MQlkpALBJY

Butylbenzylphthalate

https://spectrabase.com/spectrum/HAxqzLMKPM8

Butylbenzylphthalate

https://spectrabase.com/spectrum/1s5iYgiKwbY

Butylbenzylphthalate

https://spectrabase.com/spectrum/8weUE3o7Bw

Butylbenzylphthalate

https://spectrabase.com/spectrum/FTPIopBeyUy

Butylbenzylphthalate

https://spectrabase.com/spectrum/93bRl1KydwO

Butylbenzylphthalate

https://spectrabase.com/spectrum/GufvUmr3uKm

Butylbenzylphthalate

https://spectrabase.com/spectrum/4po3Yj4dc1Y

Butylbenzylphthalate

https://spectrabase.com/spectrum/Lvl4Phe1Erw

Butylbenzylphthalate

https://spectrabase.com/spectrum/LtDMze12LIm

Butylbenzylphthalate

https://spectrabase.com/spectrum/FZwADGMwB7I

Butylbenzylphthalate

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 ${\it Butylbenzylphthalate}$

https://spectrabase.com/spectrum/DlxsbMDTdCK

1-Benzyl 2-butyl phthalate

https://spectrabase.com/spectrum/G9JGZLUejrx

26. Springer Nature

27. SpringerMaterials

phthalic acid benzyl ester butyl ester

https://materials.springer.com/substanceprofile/docs/smsid_qqlsrygjkrnkeuff

28. The National Institute for Occupational Safety and Health (NIOSH)

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Phthalic acid, benzyl butyl ester

https://www.cdc.gov/niosh-rtecs/TH986F70.html

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https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

Butyl Benzyl Phthalate

https://epa-prgs.ornl.gov/cgi-bin/chemicals/csl_search

Butyl Benzyl Phthalate

 $https://epa-prgs.ornl.gov/cgi-bin/chemicals/csl_search?tool=rml$

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benzyl butyl phthalate https://en.wikipedia.org/wiki/Benzyl_butyl_phthalate

31. PubChem

https://pubchem.ncbi.nlm.nih.gov

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butylbenzyl phthalate

https://www.ncbi.nlm.nih.gov/mesh/67027561

MeSH Tree

http://www.nlm.nih.gov/mesh/meshhome.html

Teratoaens

https://www.ncbi.nlm.nih.gov/mesh/68013723

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Endocrine disrupting compounds http://www.genome.jp/kegg-bin/get_htext?br08006.keg

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ATC Code

https://www.whocc.no/atc_ddd_index/

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GHS Classification Tree

http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

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NORMAN Suspect List Exchange Classification https://www.norman-network.com/nds/SLE/

37. PATENTSCOPE (WIPO)

SID 403030148

https://pubchem.ncbi.nlm.nih.gov/substance/403030148