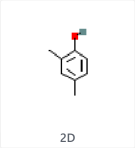
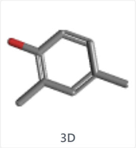
COMPOUND SUMMARY

2,4-Dimethylphenol

PubChem CID	7771
Structure	 2D  3D Find Similar Structures
Chemical Safety	Corrosive Acute Toxic Irritant Environmental Hazard Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_8H_{10}O$ or $(CH_3)_2C_6H_3OH$
Synonyms	2,4-DIMETHYLPHENOL 105-67-9 2,4-Xylenol Phenol, 2,4-dimethyl- 4,6-Dimethylphenol More...
Molecular Weight	122.16
Dates	Modify 2021-07-03 Create 2005-03-26

2,4-dimethylphenol appears as colorless crystals or clear, dark amber liquid.

- CAMEO Chemicals

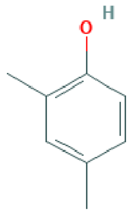
2,4-Dimethylphenol is a hydroxytoluene.

- ChEBI

1 Structures

1.1 2D Structure

Chemical Structure Depiction



PubChem

1.2 3D Conformer

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

2,4-dimethylphenol

Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)

▸ PubChem

2.1.2 InChI

InChI=1S/C8H10O/c1-6-3-4-8(9)7(2)5-6/h3-5,9H,1-2H3

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

▸ PubChem

2.1.3 InChI Key

KUFFULVDNCHOFZ-UHFFFAOYSA-N

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

▸ PubChem

2.1.4 Canonical SMILES

CC1=CC(=C(C=C1)O)C

Computed by OEChem 2.1.5 (PubChem release 2019.06.18)

▸ PubChem

2.2 Molecular Formula

$C_8H_{10}O$

▸ CAMEO Chemicals; PubChem

$C_8H_{10}O$

$(CH_3)_2C_6H_3OH$

▸ ILO International Chemical Safety Cards (ICSC)

2.3 Other Identifiers

2.3.1 CAS

105-67-9

▸ 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); The National Institute for Occupational Safety and Health

2.3.2 European Community (EC) Number

203-321-6

▸ European Chemicals Agency (ECHA)

2.3.3 ICSC Number

0458

- ILO International Chemical Safety Cards (ICSC)

2.3.4 NSC Number

3829

- DTP/NCI

2.3.5 RTECS Number

ZE5600000

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

2.3.6 UN Number

2261

- CAMEO Chemicals; ILO International Chemical Safety Cards (ICSC)

3082

- NJDOH RTK Hazardous Substance List

2.3.7 UNII

5OD803C081

- FDA/SPL Indexing Data

2.3.8 DSSTox Substance ID

DTXSID2021864

- EPA DSSTox

2.3.9 Wikipedia

2,4-Dimethylphenol

- Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

2,4-dimethylphenol
2,4-dimethylphenol potassium
2,4-dimethylphenol sodium
2,4-dimethylphenol titanium (+4)
2,4-DMP
2,4-xylenol

- Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

2,4-DIMETHYLPHENOL
105-67-9
2,4-Xylenol
Phenol, 2,4-dimethyl-
4,6-Dimethylphenol
1-Hydroxy-2,4-dimethylbenzene
4-Hydroxy-1,3-dimethylbenzene
RCRA waste number U101
2,4-Dimethyl phenol
NSC 3829
UNII-5OD803C081
2,4-Dimethyl-phenol
CHEBI:34241
5OD803C081
DSSTox_CID_1864
DSSTox_RID_76371
DSSTox_GSID_21864
Caswell No. 907A
Lysol Brand disinfectant
CAS-105-67-9
Bulk Lysol Brand Disinfectant
CCRIS 721
HSDB 4253
2,4-DMP
Gable-Tite Dark Creosote (Creola)
Benzene, 2,4-dimethyl-1-hydroxy-
Du Cor Concentrated Fly Insecticide
Gable-Tite Light Creosote (Creola)
EINECS 203-321-6
RCRA waste no. U101
EPA Pesticide Chemical Code 086804
BRN 0636244
AI3-17612
2,4dimethylphenol
2.4-dimethylphenol
PubChem21747
ACMC-1BSNQ
EC 203-321-6
SCHEMBL92167
2,4-Dimethylphenol, 98%
4-06-00-03126 (Beilstein Handbook Reference)
MLS002152861
BIDD:ER0275
CHEMBL29878
WLN: QR B1 D1
1,3-Dimethyl-4-hydroxybenzene
2,4-Xylenol, >=98%
DTXSID2021864
NSC3829
2,4-Dimethylphenol 2,4-Xylenol
HMS3039J10
ACT00460
NSC-3829
ZINC1672873
Tox21_201787
Tox21_300051
ANW-15264
BBL011443
MFCD00002233
SBB060657
STL146554
AKOS000121556
AM62796
MCULE-2639440236
2,4-Dimethylphenol, analytical standard
NCGC00091611-01
NCGC00091611-02
NCGC00091611-03
NCGC00091611-04
NCGC00091611-05
NCGC00253938-01
NCGC00259336-01
L077
PS-11923
SMR001224485
DB-010714
D0774
FT-0610239
ST51046795
2,4-Dimethylphenol 100 microg/mL in Methanol
C14582
Q2437536
W-108780
2,4-Dimethylphenol, PESTANAL(R), analytical standard

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	122.16	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3	2.3	Computed by XLogP3 3.0 (PubChem release 2019.06.18)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	1	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Rotatable Bond Count	0	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	122.073164938	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	122.073164938	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	20.2 Å^2	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	9	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	90.6	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

2,4-dimethylphenol appears as colorless crystals or clear, dark amber liquid.

▸ CAMEO Chemicals

Liquid

▸ EPA Chemicals under the TSCA

YELLOW-TO-BROWN LIQUID OR COLOURLESS CRYSTALS.

▸ ILO International Chemical Safety Cards (ICSC)

3.2.2 Color/Form

Crystals

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1723

▸ Hazardous Substances Data Bank (HSDB)

NEEDLES FROM WATER

Weast, R.C. (ed.) Handbook of Chemistry and Physics. 69th ed. Boca Raton, FL: CRC Press Inc., 1988-1989., p. C-411

▸ Hazardous Substances Data Bank (HSDB)

Colorless needles

Verschueren, K. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York, NY: Van Nostrand Reinhold Co., 1996., p. 1902

▸ Hazardous Substances Data Bank (HSDB)

3.2.3 Taste

0.5 mg/l (taste threshold concn)

Verschueren, K. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York, NY: Van Nostrand Reinhold Co., 1996., p. 1902

▸ Hazardous Substances Data Bank (HSDB)

3.2.4 Boiling Point

414 °F at 766 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

210.9 °C

▸ EPA DSSTox

211.5 °C @ 766 mm Hg; 210.8 @ 760 mm Hg

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1723

▸ Hazardous Substances Data Bank (HSDB)

211.5 °C

▸ ILO International Chemical Safety Cards (ICSC)

3.2.5 Melting Point

72 to 73 °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

24.5 °C

▸ EPA DSSTox

25.4-26 °C; 24.54 °C

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1723

▸ Hazardous Substances Data Bank (HSDB)

25.4-26 °C

▸ ILO International Chemical Safety Cards (ICSC)

3.2.6 Flash Point

greater than 235 °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

>112 °C (closed cup)

Dean, J.A. Handbook of Organic Chemistry. New York, NY: McGraw-Hill Book Co., 1987., p. 1-213

▸ Hazardous Substances Data Bank (HSDB)

>112 °C c.c.

▸ ILO International Chemical Safety Cards (ICSC)

3.2.7 Solubility

less than 1 mg/mL at 64° 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

0.06 M

BANERJEE,S ET AL. (1980)

▸ EPA DSSTox

Miscible in ethyl alcohol, ethyl ether; soluble in carbon tetrachloride

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 76th ed. Boca Raton, FL: CRC Press Inc., 1995-1996., p. 3-255

▸ Hazardous Substances Data Bank (HSDB)

Very sol in benzene, chloroform

Dean, J.A. Handbook of Organic Chemistry. New York, NY: McGraw-Hill Book Co., 1987., p. 1-213

▸ Hazardous Substances Data Bank (HSDB)

In water, 7.87X10+3 mg/l @ 25 °C.

Yalkowsky SH, Dannenfelser RM; The AQUASOL dATAbASE of Aqueous Solubility. Fifth ed, Tucson, AZ: Univ Az, College of Pharmacy (1992)

▸ Hazardous Substances Data Bank (HSDB)

Soluble in oxygenated and aromatic solvents

Ashford, R.D. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., 1994., p. 956

▸ Hazardous Substances Data Bank (HSDB)

7.2 x 10 (-2) mol/l, at pH 5.1 and 25 °C.

Blackman GE et al; Arch Biochem Biophys 54: 55-71 (1955)

▸ Hazardous Substances Data Bank (HSDB)

Solubility in water, g/100ml at 25 °C: 0.79

▸ ILO International Chemical Safety Cards (ICSC)

3.2.8 Density

1.0276 at 57 °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

0.9650 @ 20 °C/4 °C

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 76th ed. Boca Raton, FL: CRC Press Inc., 1995-1996., p. 3-255

▸ Hazardous Substances Data Bank (HSDB)

0.97 g/cm^3

- ILO International Chemical Safety Cards (ICSC)

3.2.9 Vapor Pressure

0.0621 mm Hg at 68 °F ; 1 mm Hg at 125.2° 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

0.10 mmHg

- EPA DSSTox

0.102 mm Hg @ 25 °C

Daubert, T.E., R.P. Danner. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis, 1989.

- Hazardous Substances Data Bank (HSDB)

Vapor pressure, Pa at 20 °C: 8

- ILO International Chemical Safety Cards (ICSC)

3.2.10 LogP

2.3 (LogP)

HANSCH,C ET AL. (1995)

- EPA DSSTox

log Kow= 2.30

Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995., p. 44

- Hazardous Substances Data Bank (HSDB)

2.3

- ILO International Chemical Safety Cards (ICSC)

3.2.11 Henrys Law Constant

9.51e-07 atm-m3/mole

- EPA DSSTox

Henry's Law constant = 1.7X10-5 atm-cu m/mol @ 25 °C

Smith JR et al; Water Environ Res 65: 804-18 (1993)

- Hazardous Substances Data Bank (HSDB)

3.2.12 Atmospheric OH Rate Constant

7.15e-11 cm3/molecule*sec

KWOK,ESC & ATKINSON,R (1994)

- EPA DSSTox

3.2.13 Autoignition Temperature

599 °C

- ILO International Chemical Safety Cards (ICSC)

3.2.14 Decomposition

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

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 3406

- Hazardous Substances Data Bank (HSDB)

3.2.15 Heat of Vaporization

64.96 kJ/mole @ 210.98 °C

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 76th ed. Boca Raton, FL: CRC Press Inc., 1995-1996., p. 6-124

- Hazardous Substances Data Bank (HSDB)

3.2.16 Odor Threshold

0.001 mg/cu m (recognition in air); 0.0005-0.4 mg/cu m (detection in air)

Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983., p. 1195

- Hazardous Substances Data Bank (HSDB)

0.4 mg/l (detection in water)

Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983., p. 1196

- Hazardous Substances Data Bank (HSDB)

3.2.17 Refractive Index

Index of refraction: 1.5420 @ 14 °C/D

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 76th ed. Boca Raton, FL: CRC Press Inc., 1995-1996., p. 3-255

- Hazardous Substances Data Bank (HSDB)

3.2.18 Dissociation Constants

pKa= 10.60 at 25 °C

Serjeant EP, Dempsey B; Ionisation constants of organic acids in aqueous solution. IUPAC Chem Data Ser No.23. NY,NY: Pergamon pp. 989 (1979)

- Hazardous Substances Data Bank (HSDB)

3.2.19 Kovats Retention Index

Standard non-polar	1123, 1123, 1133, 1135, 1124, 1126, 1126, 1127, 1094, 1094, 1130, 1132, 1162, 1134, 1177, 1126, 1126, 1120, 1123, 1123, 1127, 1134, 1120, 1121.6, 1087, 1123, 1123, 1134
Semi-standard non-polar	1148.9, 1150.1, 1151.4, 1160, 1148.3, 1150, 1150, 1128, 1172, 1181, 1144, 1145, 1150, 1154, 1156, 1149, 1162.3, 1154.1, 1149, 1150, 1151, 192.24, 190.9, 191.2, 192.69
Standard polar	2078, 2073, 2090, 2094.74, 2098.02, 2098.97, 2098.99, 2087, 2079, 2070, 2078, 2058.1, 2127, 2050.4

- NIST Mass Spectrometry Data Center

3.2.20 Other Experimental Properties

Dipole moment: 1.48 debyes (benzene, 20 °C); 1.98 debyes (benzene, 60 °C)

Dean, J.A. Handbook of Organic Chemistry. New York, NY: McGraw-Hill Book Co., 1987., p. 4-58

- Hazardous Substances Data Bank (HSDB)

Hydroxyl radical rate constant = 7.20X10-11 cu-cm/molc sec @ 25 °C

Atkinson R; J Phys Chem Ref Data. Monograph 2 (1994)

▸ Hazardous Substances Data Bank (HSDB)

3.3 SpringerMaterials Properties

- 13C nuclear magnetic resonance spectrum
- Boiling point
- Chemical diffusion
- Chemical shift
- Density
- Diamagnetic susceptibility
- Dielectric constant
- Diffusion
- Diffusive flux
- Heat of sublimation
- Magnetic susceptibility
- Optical coefficient
- Phase diagram
- Phase equilibrium
- Refractive index
- Spin-spin coupling constant
- Surface tension
- Thermal expansion coefficient
- Vapor pressure
- Vapor-liquid equilibrium

▸ SpringerMaterials

4 Spectral Information

4.1 1D NMR Spectra

1D NMR Spectra	NMR: 6016 (Sadtler Research Laboratories Spectral Collection)

Hazardous Substances Data Bank (HSDB)

4.1.1 1H NMR Spectra

Instrument Name	Varian A-60
Source of Sample	Aldrich Chemical Company, Inc., Milwaukee, Wisconsin
Copyright	Copyright © 2009-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

4.1.2 13C NMR Spectra

Showing 2 of 20 View More

Source of Sample	Eastman Organic Chemicals, Rochester, New York
Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

Copyright	Copyright © 2016-2020 W. Robien, Inst. of Org. Chem., Univ. of Vienna. All Rights Reserved.
Thumbnail	

SpectraBase

4.2 Mass Spectrometry

Showing 2 of 12 View More

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	

SpectraBase

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 7 View More

MoNA ID	JP000018
MS Category	Experimental
MS Type	GC-MS
MS Level	MS1
Instrument	VARIAN MAT-44
Instrument Type	EI-B
Ionization Mode	positive
Top 5 Peaks	107 100 122 80.7 121 65.1 77 36.1 106 27.2
SPLASH	splash10-05fr-6900000000-a95cb4f62c467e4d09c0
Thumbnail	
Submitter	University of Tokyo Team, Faculty of Engineering, University of Tokyo

MassBank of North America (MoNA)

MoNA ID	JP004035
MS Category	Experimental
MS Type	GC-MS
MS Level	MS1
Instrument	HITACHI RMU-6L
Instrument Type	EI-B
Ionization Mode	positive

Top 5 Peaks	122 100 107 88.9 121 55.5 39 26.0 91 18.1
SPLASH	splash10-05fr-5900000000-b92f4c08331c6a417dc9
Thumbnail	
Submitter	University of Tokyo Team, Faculty of Engineering, University of Tokyo

▸ MassBank of North America (MoNA)

4.2.2 Other MS

Other MS	MASS: 201 (National Bureau of Standards EPA-NIH Mass Spectra Data Base, NSRDS-NBS-63)
Other MS	MASS: 507 (Atlas of Mass Spectral Data, John Wiley & Sons, New York)

▸ Hazardous Substances Data Bank (HSDB)

4.3 UV Spectra

MAX ABSORPTION (CYCLOHEXANE): 280 NM (LOG E= 3.31)

Weast, R.C. (ed.). Handbook of Chemistry and Physics. 60th ed. Boca Raton, Florida: CRC Press Inc., 1979., p. C-162

▸ Hazardous Substances Data Bank (HSDB)

UV: 178 (Sadtler Research Laboratories Spectral Collection)

Weast, R.C. and M.J. Astle. CRC Handbook of Data on Organic Compounds. Volumes I and II. Boca Raton, FL: CRC Press Inc. 1985., p. V2 62

▸ Hazardous Substances Data Bank (HSDB)

4.4 IR Spectra

IR Spectra	IR: 15054 (Sadtler Research Laboratories IR Grating Collection)

▸ Hazardous Substances Data Bank (HSDB)

4.4.1 FTIR Spectra

Showing 2 of 9 View More

Technique	BETWEEN SALTS
Source of Sample	Bridgestone/Firestone, Inc.

Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

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

SpectraBase

4.4.2 ATR-IR Spectra

Showing 2 of 4 View More

Technique	ATR-Cylindrical Internal Reflectance (CIR)
Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

▸ SpectraBase

Instrument Name	Bruker Tensor 27 FT-IR
Technique	ATR-Neat (DuraSamplIR II)
Source of Spectrum	Bio-Rad Laboratories, Inc.
Source of Sample	Alfa Aesar, Thermo Fisher Scientific
Catalog Number	A11966
Lot Number	10165155
Copyright	Copyright © 2016-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

▸ SpectraBase

4.4.3 Near IR Spectra

Technique	NIR Path Length= 0.5/20 (20 = 4.5 mm) Spectrometer= BRUKER IFS 88 Spectrometer= INSTRUMENT PARAMETERS=INST=BRUKER,RSN=11126,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	

SpectraBase

Technique	NIR Path Length= 0.5/20 (20 = 4.5 mm) Spectrometer= BRUKER IFS 88 Spectrometer= INSTRUMENT PARAMETERS=INST=BRUKER,RSN=11126,REO=2,CNM=HEI,ZFF=2
Source of Spectrum	Prof. Buback, University of Goettingen, Germany
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Thumbnail	

SpectraBase

4.4.4 Vapor Phase IR Spectra

Technique	Vapor Phase
Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

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	

SpectraBase

4.5 Raman Spectra

Instrument Name	Bruker MultiRAM Stand Alone FT-Raman Spectrometer
Technique	FT-Raman
Source of Spectrum	Bio-Rad Laboratories, Inc.
Source of Sample	Alfa Aesar, Thermo Fisher Scientific
Catalog Number	A11966
Lot Number	10165155
Copyright	Copyright © 2016-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

Catalog Number	D174203
Copyright	Copyright © 2017-2020 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2017-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

▸ SpectraBase

5 Related Records

5.1 Related Compounds with Annotation

▸ PubChem

5.2 Related Compounds

Same Connectivity	4 Records
Same Parent, Connectivity	55 Records
Same Parent, Exact	52 Records
Mixtures, Components, and Neutralized Forms	169 Records
Similar Compounds	6,339 Records
Similar Conformers	8,894 Records

▸ PubChem

5.3 Substances

5.3.1 Related Substances

All	374 Records
Same	167 Records
Mixture	207 Records

▸ PubChem

5.3.2 Substances by Category

▸ PubChem

5.4 Entrez Crosslinks

PubMed	307 Records
Protein Structures	1 Record
Taxonomy	1 Record
Gene	2 Records

▸ PubChem

6 Chemical Vendors

▸ PubChem

7 Drug and Medication Information

7.1 Maximum Drug Dose

The lethal dose of Lysol is about 60 to 120 ml, although lesser amounts have been associated with death.

Ellenhorn, M.J., S. Schonwald, G. Ordog, J. Wasserberger. Ellenhorn's Medical Toxicology: Diagnosis and Treatment of Human Poisoning. 2nd ed. Baltimore, MD: Williams and Wilkins, 1997., p. 1211

▸ Hazardous Substances Data Bank (HSDB)

8 Food Additives and Ingredients

8.1 Food Additive Classes

Flavoring Agents

▸ EU Food Improvement Agents

9 Pharmacology and Biochemistry

9.1 Absorption, Distribution and Excretion

SUBJECTS WERE EXPOSED TO M-XYLENE AT CONCN OF ABOUT 3.9 MMOL/CU M FOR 5 DAYS, 6 HR/DAY. RATE OF 2,4-XYLENOL EXCRETION SHORTLY AFTER EXPOSURE WAS ABOUT 1-2% OF THAT FOR METHYLHIPPURIC ACID EXCRETION AND PULMONARY EXCRETION OF UNCHANGED XYLENE WAS ABOUT 4% OF UPTAKE.

RIIHIMAKI V ET AL; SCAND J WORK ENVIRON HEALTH 5 (3): 217-31 (1979)

▸ Hazardous Substances Data Bank (HSDB)

The concn of 2,4-dimethylphenol was determined /in/ several tissues of the rat after 6 hr constant iv infusion and after iv bolus injection. 2,4-dimethylphenol was distributed rapidly in the brain and liver, /and had/ high tissue-plasma concn ratios for the brain, liver, and fat. Accumulation of 2,4-dimethylphenol in these tissues was negligible.

PMID:7067652
Kata JS et al; Ecotoxicol Environ Saf 6 (1): 35-40 (1982)

▸ Hazardous Substances Data Bank (HSDB)

FOLLOWING IV ADMIN OF 17 MG/KG OF THE 2,4-ISOMER TO RATS, THE BRAIN ACCUMULATED THE HIGHEST AMT ON A PER G BASIS, FOLLOWED BY FAT AND LIVER. RATIOS OF BRAIN, LIVER AND FAT TO PLASMA /CONCN/ WERE APPROX 1, 1.5 AND 2, RESPECTIVELY.

SOMANI SM; FED PROC FED AM SOC EXP BIOL 40 (3PT1): 698 (1981)

▸ Hazardous Substances Data Bank (HSDB)

2,4-DIMETHYLPHENOL DISTRIBUTED RAPIDLY THROUGH THE BODY AFTER IV BOLUS ADMIN OF 30 MG/KG. PLASMA, LIVER AND FAT CONCN DISAPPEARED PRIOR TO 60 MIN BUT PERSISTED IN THE BRAIN.

SOMANI SM; FED PROC FED AM SOC EXP BIOL 40 (3PT1): 698 (1981)

▸ Hazardous Substances Data Bank (HSDB)

Associations between o-cresol, p-cresol, m-cresol, 2,4-xylenol, 2,5-xylenol, 3,4-xylenol, and 3,5-xylenol exposure levels and urinary phenol excretion were examined in the coke facility industry. The subjects consisted of 76 exposed workers employed in the tar distillation process and 34 controls. ... Urinary metabolite levels were corrected for specific gravity and creatinine. The time weighted average exposure concentrations in the breathing zones of the tar distillation workers were ... 0.02 to 0.04 mg/cu m for xylenols. ... The urinary xylenol levels of exposed workers ranged from 0.12 to 0.97 mg/l with specific gravity correction. In control urine samples, the specific gravity corrected xylenol concentrations ranged from 25 x 10(-3) to 43 x 10(-3) mg/l. Significant correlations were observed between the ambient levels and urinary concentrations of phenol, o-cresol, and the xylenols, with coefficients ranging from 0.45 to 0.82. The author concludes that the biological monitoring of urinary xylenols may be used as a means of measuring xylenol exposure in coke facility workers.

PMID:9352337
Bieniek G; International Archives of Occupational and Environmental Health 70 (5): 334-40 (1997)

▸ Hazardous Substances Data Bank (HSDB)

9.2 Metabolism/Metabolites

METABOLISM OF 2,4-DIMETHYLPHENOL IN ANIMALS IS VERY SIMILAR TO THAT OF CRESOLS ... .

National Research Council. Drinking Water & Health Volume 1. Washington, DC: National Academy Press, 1977., p. 730

▸ Hazardous Substances Data Bank (HSDB)

Rats were admin 2,4-dimethylphenol for 6 hr constantly by iv infusion or iv bolus injection. 2,4-Dimethylphenol was rapidly metabolized to its conjugates (94.3%) within 30 min; the glucuronide constituted 53% and other conjugates 41% /in plasma/.

PMID:7067652
Kata JS et al; Ecotoxicol Environ Saf 6 (1): 35-40 (1982)

▸ Hazardous Substances Data Bank (HSDB)

IN WORKERS SIMULTANEOUSLY EXPOSED TO ETHYLBENZENES AND XYLENES, 2,4-DIMETHYLPHENOL, A METABOLITE OF M-XYLENE, COULD NOT BE DETECTED.

PMID:437902
ANGERER J, LEHNERT G; INT ARCH OCCUP ENVIRON HEALTH 43 (2): 145-50 (1979)

▸ Hazardous Substances Data Bank (HSDB)

HYDROXYLATION OF AROMATIC HYDROCARBONS WAS STUDIED FOLLOWING THEIR ORAL ADMINISTRATION TO RATS THAT ALSO RECEIVED A PURIFIED DIET CONTAINING NEOMYCIN TO REDUCE THE LEVELS OF NORMALLY OCCURRING SIMPLE URINARY PHENOLS. PHENOLIC METABOLITES WERE QUANTITATIVELY ESTIMATED IN HYDROLYZED URINE SAMPLES BY GAS CHROMATOGRAPHY. M-XYLENE ADMINISTERED AT A DOSE OF 100 MG/KG WAS METABOLIZED TO 2,4-DIMETHYLPHENOL TO THE EXTENT OF 0.9% OF THE DOSE GIVEN.

PMID:5422210
BAKKE OM, SCHELINE RR; TOXICOL APPL PHARMACOL 16 (3): 691-700 (1970)

- Hazardous Substances Data Bank (HSDB)

For more Metabolism/Metabolites (Complete) data for 2,4-DIMETHYLPHENOL (6 total), please visit the HSDB record page.

- Hazardous Substances Data Bank (HSDB)

2,4-Dimethylphenol is a known human metabolite of m-xylene.

S73 | METXBIODB | Metabolite Reaction Database from BioTransformer | DOI:10.5281/zenodo.4056560

- NORMAN Suspect List Exchange

9.3 Biochemical Reactions

- PubChem

9.4 Transformations

- NORMAN Suspect List Exchange

10 Use and Manufacturing

10.1 Use Classification

Food additives -> Flavoring Agents

▸ EU Food Improvement Agents

10.2 Household Products

Household & Commercial/Institutional Products

Information on 5 consumer products that contain 2,4-Xylenol in the following categories is provided:

• Auto Products

• Inside the Home

▸ Consumer Product Information Database (CPID)

10.3 Uses

EPA CPDat Chemical and Product Categories

▸ EPA Chemical and Products Database (CPDat)

MANUFACTURE OF PHARMACEUTICALS, PLASTICS, INSECTICIDES, FUNGICIDES, RUBBER CHEM, WETTING AGENTS, DYESTUFFS.

National Research Council. Drinking Water & Health Volume 1. Washington, DC: National Academy Press, 1977., p. 730

▸ Hazardous Substances Data Bank (HSDB)

HORTICULTURAL FORMULATION FOR ERADICATION OF CROWN GALL TUMORS.

Farm Chemicals Handbook 87. Willoughby, Ohio: Meister Publishing Co., 1987., p. C-28

▸ Hazardous Substances Data Bank (HSDB)

Used in phosphate esters, alkylated xylenols, antioxidants. /Xylenol 100/

Flick, E.W. Industrial Solvents Handbook. 3rd ed. Park Ridge, NJ: Noyes Publications, 1985., p. 368

▸ Hazardous Substances Data Bank (HSDB)

Used in the production of high-viscosity phosphate esters, as a feedstock for hindered phenol antioxidant and specialty modified phenolic resin manufacture. /Xylenol 410/

Flick, E.W. Industrial Solvents Handbook. 3rd ed. Park Ridge, NJ: Noyes Publications, 1985., p. 370

▸ Hazardous Substances Data Bank (HSDB)

For more Uses (Complete) data for 2,4-DIMETHYLPHENOL (13 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

10.3.1 Industry Uses

Intermediates
Processing aids, not otherwise listed
Solvents (for cleaning and degreasing)
Solvents (which become part of product formulation or mixture)

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

EPA Chemicals under the TSCA

10.3.2 Consumer Uses

Cleaning and furnishing care products
Paints and coatings

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

EPA Chemicals under the TSCA

10.4 Methods of Manufacturing

Coal tar fractionation; processing.

Verschueren, K. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York, NY: Van Nostrand Reinhold Co., 1996., p. 1902

Hazardous Substances Data Bank (HSDB)

The insertion of methyl groups into phenol to produce ... xylenols is a commercial process of considerable utility. The process commonly employed is methylation with methyl alcohol over a solid catalyst, generally a modified metal oxide, at temp in the range of 300-450 °C. /Xylenols/

Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. 2(78) 66

Hazardous Substances Data Bank (HSDB)

Fractionation of mixed xylenols

Ashford, R.D. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., 1994., p. 956

Hazardous Substances Data Bank (HSDB)

10.5 Formulations/Preparations

2,4-XYLENOL AND M-CRESOL IN AN EMULSIFIED FORMULATION OF HYDROCARBONS AND WATER. HORTICULTURAL FORMULATION FOR ERADICATION OF CROWN GALL TUMORS. /BACTICIN/

Farm Chemicals Handbook 88. Willoughby, Ohio: Meister Publishing Co., 1988., p. C-24

Hazardous Substances Data Bank (HSDB)

Xylenol 100; a high purity fraction of 2,4- and 2,5- xylenol (ortho xylenols); typical composition: 2,4- 2,5-xylenol 93%; meta para cresol 2%; other xylenols 5% /From table/

Flick, E.W. Industrial Solvents Handbook. 3rd ed. Park Ridge, NJ: Noyes Publications, 1985., p. 368

Hazardous Substances Data Bank (HSDB)

Pitt-Consol Xylenol 410 is a synthetic xylenol blend ... homolog distribution, wt %: 2,6-xylenol, 1; 2,4-xylenol, 42; 2,5-xylenol, 43; 2,3-xylenol group, 14. /Xylenol 410/

Flick, E.W. Industrial Solvents Handbook. 3rd ed. Park Ridge, NJ: Noyes Publications, 1985., p. 370

Hazardous Substances Data Bank (HSDB)

Bulk Lysol Brand Disinfectant, soluble concentrate, 1.5% 2,4-xylenol.

Purdue University; National Pesticide Information Retrieval System (1988)

- Hazardous Substances Data Bank (HSDB)

For more Formulations/Preparations (Complete) data for 2,4-DIMETHYLPHENOL (11 total), please visit the HSDB record page.

- Hazardous Substances Data Bank (HSDB)

10.6 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) AT LEAST 9.99X10+8 G

SRI

- Hazardous Substances Data Bank (HSDB)

10.7 U.S. Imports

(1977) AT LEAST 4.54X10+7 G

SRI

- Hazardous Substances Data Bank (HSDB)

(1982) 5.28X10+7 G (PRINCIPAL CUSTOMS DISTRICTS)

SRI

- Hazardous Substances Data Bank (HSDB)

(1983) 1.06X10+8 g

USITC. IMPORTS OF BENZENOID CHEM & PROD p.30 (1983)

- Hazardous Substances Data Bank (HSDB)

10.8 General Manufacturing Information

Industry Processing Sectors

All other basic organic chemical manufacturing
All other chemical product and preparation manufacturing
Mining (except oil and gas) and support activities
Paint and coating manufacturing
Plastic material and resin manufacturing
Soap, cleaning compound, and toilet preparation manufacturing

- EPA Chemicals under the TSCA

EPA TSCA Commercial Activity Status

Phenol, 2,4-dimethyl-: ACTIVE

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

- EPA Chemicals under the TSCA

ISOMERIZATION OF 1,4-DIMETHYLBENZENE OXIDE TO 2,4-DIMETHYLPHENOL WAS ANALOGOUS TO METHYL MIGRATION IN ENZYMIC CONVERSION OF 4-METHYLPHENYLALANINE TO 3-METHYLTYROSINE WITH PHENYLALANINE HYDROXYLASE.

JERINA DM ET AL; PROC NAT ACAD SCI US 68 (10): 2545-8 (1971)

- Hazardous Substances Data Bank (HSDB)

Discontinued by TUCO, Division of the Upjohn Co. /Bacticin/

Farm Chemicals Handbook 88. Willoughby, Ohio: Meister Publishing Co., 1988., p. C-24

- Hazardous Substances Data Bank (HSDB)

10.9 Sampling Procedures

TRACES OF PHENOLS (INCLUDING 2,4-DIMETHYLPHENOL) IN AUTO EXHAUST AND TOBACCO SMOKE WERE COLLECTED USING A FRITTED BUBBLER WITH 10 ML 0.12% SODIUM HYDROXIDE SOLUTION.

KUWATA K ET AL; ANAL CHEM 53 (9): 1531-4 (1981)

- Hazardous Substances Data Bank (HSDB)

EPA Method 8040: Phenols. For the detection of phenolic compounds, a representative sample (solid or liquid) is collected in a glass container equipped with a Teflon-lined cap.

USEPA; Test Methods for Evaluating Solid Waste SW-846 (1986)

- Hazardous Substances Data Bank (HSDB)

11 Identification

11.1 Analytic Laboratory Methods

SEPARATION OF 13 ISOMERIC ALKYLPHENOLS WAS STUDIED BY HIGH PERFORMANCE LIQUID (HPLC), GAS LIQUID (GLC), & HIGH PERFORMANCE THIN LAYER CHROMATOGRAPHY (HPTLC) TECHNIQUES. /ALKYLPHENOLS/

HUSAIN S ET AL; J CHROMATOGR 137 (1): 53-60 (1977)

▸ Hazardous Substances Data Bank (HSDB)

A SEPARATION TECHNIQUE WAS DEVELOPED USING REVERSE PHASE HIGH PRESSURE LIQ CHROMATOGRAPHY TO ISOLATE CHEMICALS HAVING POTENTIALLY HIGH LIPID WATER PARTITION COEFFICIENTS. RETENTION VOLUME DATA FOR SELECTED CHEMICALS USING THIS METHOD FOR ANALYSIS IS PRESENTED. DATA ARE GIVEN FOR 2,4-DIMETHYLPHENOL.

VEITH GD, AUSTIN NM; IN: IDENTIFICATION & ANALYSIS OF ORGANIC POLLUTANTS IN WATER, KEITH LH, ED (ANN ARBOR: ANN ARBOR SCIENCE): 297-302 (1977)

▸ Hazardous Substances Data Bank (HSDB)

High performance liquid chromatography separation by isocratic elution of a wide range of substituted phenols, including the priority pollutant, 2,4-dimethylphenol, was investigated.

Buckman NG et al; J Chromatogr 284 (2): 441-6 (1984)

▸ Hazardous Substances Data Bank (HSDB)

A gas liquid chromatography procedure is described for identification of 32 substituted phenols. This method involves a simple and reproducible derivatization step which forms stable phenol pentafluorobenzyl ethers for which the electron capture detector is highly sensitive. Gas liquid chromatogrphy retention time data of the derivatives on 6 packed and fused silica capillary columns are reported. The detection limits using fused silica capillary columns of all chloro-, alkyl- and mononitro-phenols studied are between 0.5 and 5 picograms. /Substituted phenols/

Lee HB, Chau AS; J Assoc Off Anal Chem 66 (4): 1029-38 (1983)

▸ Hazardous Substances Data Bank (HSDB)

For more Analytic Laboratory Methods (Complete) data for 2,4-DIMETHYLPHENOL (23 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

11.2 Clinical Laboratory Methods

A sensitive and reliable procedure is described for the detection of 10 most important phenolic metabolites of benzene, toluene, xylenes and ethylbenzene. The urine was acidified with sulfuric acid and steam distilled was performed on a fused silica capillary (SE 54; 30 m) with FID. 3-Ethylphenol was used as internal standard. For phenol; o-cresol and p-cresol; DL-1- and 2-phenylethanol; 3-methylbenzylalc, 2-ethylphenol; 2,4-, 2,3-, 3,4-dimethylphenol, within series relative derivation was 2.3-16.8%. The recovery rates were 89-109%. The detection limit was 0.3 mg/l. Linearity was tested .ltoreq.50 mg/l.

Heinrich R, Angerer J; Fresenius' Z Anal Chem 322 (8): 766-71 (1985)

▸ Hazardous Substances Data Bank (HSDB)

Four methods were developed for determining minor metabolites of ethylbenzene and xylene in the urine. Methods were developed for determining 1-phenylethanol, omega-hydroxyacetophenone, 4-ethylphenol, 2,4-dimethylphenol, and 3-methylbenzyl alcohol. Following pretreatment of the sample, metabolites were determined using gas liquid chromatography and a flame ionization detector. Either acid or enzymatic hydrolysis was used as treatment and the hydrolysates were extracted with dichloromethane or diethylether.

PMID:6206558
Engstrom KM; Scand J Work Environ Health 10 (2): 75-81 (1984)

▸ Hazardous Substances Data Bank (HSDB)

/Gas chromatographic determination of urinary phenol conjugates after acid hydrolysis/extractive acetylation./ A simple gas chromatographic procedure for determining phenols in urine was developed. ... Using 10 mg/l spikes of phenol, 2-methylphenol, 3-methylphenol, 4-methylphenol, 2,6-dimethylphenol, 2,5-dimethylphenol, 2,4-dimethylphenol, 3,5-dimethylphenol, 2,3-dimethylphenol, and 3,4-dimethylphenol yielded recoveries of 94.6 to 98.2%. ...

PMID:1618971
Weber L; Journal of Chromatography 574 (2): 349-51 (1992)

▸ Hazardous Substances Data Bank (HSDB)

12 Safety and Hazards

12.1 Hazards Identification

12.1.1 GHS Classification

Showing 1 of 4 View More

Pictogram(s)	 Corrosive Acute Toxic Irritant Environmental Hazard
Signal	Danger
GHS Hazard Statements	H301 (98.99%): Toxic if swallowed [Danger Acute toxicity, oral] H311 (98.99%): Toxic in contact with skin [Danger Acute toxicity, dermal] H314 (100%): Causes severe skin burns and eye damage [Danger Skin corrosion/irritation] H317 (34%): May cause an allergic skin reaction [Warning Sensitization, Skin] H318 (35.61%): Causes serious eye damage [Danger Serious eye damage/eye irritation] H411 (99.8%): Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P260, P261, P264, P270, P272, P273, P280, P301+P310, P301+P330+P331, P302+P352, P303+P361+P353, P304+P340, P305+P351+P338, P310, P312, P321, P322, P330, P333+P313, P361, P363, P391, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided by 497 companies from 15 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

▸ European Chemicals Agency (ECHA)

12.1.2 Hazard Classes and Categories

Showing 2 of 4 View More

Acute Tox. 3 (98.99%)

Acute Tox. 3 (98.99%)

Skin Corr. 1B (100%)

Skin Sens. 1 (34%)

Eye Dam. 1 (35.61%)

Aquatic Chronic 2 (99.8%)

▸ European Chemicals Agency (ECHA)

Acute toxicity - category 3

Acute toxicity - category 3

Skin corrosion - category 1B

Hazardous to the aquatic environment (chronic) - category 2

▸ Hazardous Chemical Information System (HCIS), Safe Work Australia

12.1.3 Health Hazards

SYMPTOMS: Symptoms of exposure to this compound may include severe irritation of the skin and eyes, dizziness, stomach pain, exhaustion and damage to the liver and kidneys. Other symptoms include headache, nausea and vomiting. It may cause severe burns of the eyes and skin, irritation of the respiratory tract and coma. It may also cause corrosion of tissue of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may result in burning sensation, coughing, wheezing, laryngitis and short ness of breath. Inhalation may be fatal as a result of spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis and pulmonary edema. Symptoms of exposure to this class of compounds include profuse sweating, skin sensitization, painless blanching or erythema of the skin, intense thirst diarrhea, cyanosis from methemoglobinemia, hyperactivity, stupor, fall in blood pressure, hyperpnea, abdominal pain, hemolysis and convulsions. If death from respiratory failure is not immediate, jaundice and oliguria or anuria may occur. ACUTE/CHRONIC HAZARDS: This compound is highly toxic by ingestion, inhalation or skin absorption. It is a severe irritant of the skin and eyes. It is corrosive to the skin, eyes, mucous membranes and upper respiratory tract. When heated to decomposition it emits acrid smoke, irritating fumes and toxic fumes of carbon monoxide and carbon dioxide. (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

12.1.4 Fire Hazards

This chemical is probably combustible. (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

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

▸ ILO International Chemical Safety Cards (ICSC)

12.1.5 EPA Hazardous Waste Number

U101; A toxic waste when a discarded commercial chemical product or manufacturing chemical intermediate or an off-specification commercial chemical product or a manufacturing chemical intermediate.

▸ Hazardous Substances Data Bank (HSDB)

12.2 Safety and Hazard Properties

12.2.1 Explosive Limits and Potential

Explosive limits , vol% in air: 1.1-6.4

▸ ILO International Chemical Safety Cards (ICSC)

12.3 First Aid Measures

12.3.1 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. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. 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. Phenols are very toxic poisons AND corrosive and irritating, so that inducing vomiting may make medical problems worse. IMMEDIATELY call a hospital or poison control center and locate activated charcoal, egg whites, or milk in case the medical advisor recommends administering one of them. If advice from a physician is not readily available and the victim is conscious and not convulsing, give the victim a glass of activated charcoal slurry in water or, if this is not available, a glass of milk, or beaten egg whites and IMMEDIATELY transport victim to a hospital. If the victim is convulsing or unconscious, do not give anything by mouth, assure 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. (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

12.3.2 Inhalation First Aid

Fresh air, rest. Half-upright position. Artificial respiration may be needed. Refer for medical attention.

▸ ILO International Chemical Safety Cards (ICSC)

12.3.3 Skin First Aid

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

- ILO International Chemical Safety Cards (ICSC)

12.3.4 Eye First Aid

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)

12.3.5 Ingestion First Aid

Rinse mouth. Give one or two glasses of water to drink. Do NOT induce vomiting. Refer for medical attention .

- ILO International Chemical Safety Cards (ICSC)

12.4 Fire Fighting

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. (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

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

- ILO International Chemical Safety Cards (ICSC)

12.5 Accidental Release Measures

12.5.1 Isolation and Evacuation

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]: 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

12.5.2 Spillage Disposal

Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations. If liquid: collect leaking liquid in covered plastic containers.

- ILO International Chemical Safety Cards (ICSC)

12.5.3 Cleanup Methods

FOUNDRY PLANT WASTE GASES WERE DEODORIZED WITH POTASSIUM PERMANGANATE, AND DEODORIZATION EFFICIENCY WAS MEASURED BY PRESENCE OF 2,4-XYLENOL IN SCRUBBED WASTE GASES.

MIZUTANI H, KAMIGA K; AKUSHU NO KENYU 10 (47): 28-33 (1981)

- Hazardous Substances Data Bank (HSDB)

12.5.4 Disposal Methods

Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste number U101, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

40 CFR 240-280, 300-306, 702-799 (7/1/97)

- Hazardous Substances Data Bank (HSDB)

A good candidate for rotary kiln incineration at a temperature range of 820 to 1,600 °C and residence times of seconds for liquids and gases, and hours for solids. A good candidate for fluidized bed incineration at a temperature range of 450 to 980 °C and residence times of seconds for liquids and gases, and longer for solids.

USEPA; Engineering Handbook for Hazardous Waste Incineration p.3-13 (1981) EPA 68-03-3025

▸ Hazardous Substances Data Bank (HSDB)

A pilot plant study was conducted to evaluate the fate and behavior of 22 toxic organic compounds in conventional activated sludge wastewater treatment plants. The organic cmpd, 2,4-dimethylphenol, spiked at a nominal concn of 50 ug/l was about 99% removable. Results showed that biodegradability was variable and was a function of molecular structure.

Petrasek AC et al; J Water Pollut Control Fed 55 (10): 1286-96 (1983)

▸ Hazardous Substances Data Bank (HSDB)

The effectiveness of anaerobic filters containing granular activated carbon in treating synthetically prepared wastewaters that contained phenols, polycyclic hydroxy compounds, monocyclic N-aromatics, polycyclic N-aromatics, & aliphatic acids was evaluated. The ability of the activated carbon to retain these compounds along with its external surface, which provides vast sheltered microbial attachment areas, renders activated carbon a very unique medium for anaerobic filter treatment of coal gasification wastewater.

Suidan MT et al; J Water Pollut Control Fed 55 (10): 1263-70 (1983)

▸ Hazardous Substances Data Bank (HSDB)

For more Disposal Methods (Complete) data for 2,4-DIMETHYLPHENOL (6 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

12.5.5 Preventive Measures

Smoking, eating, and drinking before washing should be absolutely prohibited when any pesticide ... is being handled or used. /Pesticides/

International Labour Office. Encyclopedia of Occupational Health and Safety. Vols. I&II. Geneva, Switzerland: International Labour Office, 1983., p. 1617

▸ Hazardous Substances Data Bank (HSDB)

12.6 Handling and Storage

12.6.1 Nonfire Spill Response

SMALL SPILLS AND LEAKAGE: If you spill this chemical, FIRST REMOVE ALL SOURCES OF IGNITION. Then, use absorbent paper to pick up all liquid spill material. Your contaminated clothing and absorbent paper should be sealed in a vapor-tight plastic bag for eventual disposal. Solvent wash all contaminated surfaces with 60-70% ethanol followed by washing with a soap and water solution. Do not reenter the contaminated area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned. STORAGE PRECAUTIONS: You should store this chemical under ambient temperatures, and protect it from moisture and oxidizing materials. If possible, it would be prudent to store this compound under inert atmosphere. (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

12.6.2 Safe Storage

Separated from food and feedstuffs, acid anhydrides, acid chlorides, bases and oxidants.

▸ ILO International Chemical Safety Cards (ICSC)

12.6.3 Storage Conditions

Rooms used for storage only should be soundly constructed and fitted with secure locks. Floors should be kept clear, and the pesticides clearly identified. /Pesticides/

International Labour Office. Encyclopedia of Occupational Health and Safety. Vols. I&II. Geneva, Switzerland: International Labour Office, 1983., p. 1617

▸ Hazardous Substances Data Bank (HSDB)

12.7 Exposure Control and Personal Protection

12.7.1 Threshold Limit Values (TLV)

(inhalable fraction and vapour): 1 ppm as TWA; (DSEN); A3 (confirmed animal carcinogen with unknown relevance to humans)

- ILO International Chemical Safety Cards (ICSC)

12.7.2 Inhalation Risk

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20 °C.

- ILO International Chemical Safety Cards (ICSC)

12.7.3 Effects of Short Term Exposure

The substance is corrosive to the skin, respiratory tract and eyes. Corrosive on ingestion. Inhalation of the aerosol may cause lung oedema.

- ILO International Chemical Safety Cards (ICSC)

12.7.4 Effects of Long Term Exposure

Repeated or prolonged contact may cause skin sensitization.

- ILO International Chemical Safety Cards (ICSC)

12.7.5 Personal Protective Equipment (PPE)

MINIMUM PROTECTIVE CLOTHING: If Tyvek-type disposable protective clothing is not worn during handling of this chemical, wear disposable Tyvek-type sleeves taped to your gloves. RECOMMENDED RESPIRATOR: Where the neat test chemical is weighed and diluted, wear a NIOSH-approved half face respirator equipped with an organic vapor/acid gas cartridge (specific for organic vapors, HCl, acid gas and SO2) with a dust/mist filter. (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

Some data suggesting breakthrough times /for butyl rubber/ of approximately an hour or more. /Aromatic hydroxyl cmpd/

ACGIH; Guidelines Select of Chem Protect Clothing Volume #1 Field Guide p.78 (1983)

- Hazardous Substances Data Bank (HSDB)

Breakthrough times /for neoprene/ greater than one hour reported by (normally) two or more testers. /Aromatic hydroxyl cmpd/

ACGIH; Guidelines Select of Chem Protect Clothing Volume #1 Field Guide p.78 (1983)

- Hazardous Substances Data Bank (HSDB)

Breakthrough times /for polyvinyl alcohol/ less (usually ... /markedly/ less) than one hour reported by (normally) two or more testers. /Aromatic hydroxyl cmpd/

ACGIH; Guidelines Select of Chem Protect Clothing Volume #1 Field Guide p.78 (1983)

- Hazardous Substances Data Bank (HSDB)

12.7.6 Fire Prevention

NO open flames.

- ILO International Chemical Safety Cards (ICSC)

12.7.7 Exposure Prevention

PREVENT DISPERSION OF DUST! PREVENT GENERATION OF MISTS! STRICT HYGIENE!

- ILO International Chemical Safety Cards (ICSC)

12.7.8 Inhalation Prevention

Use ventilation, local exhaust or breathing protection.

- ILO International Chemical Safety Cards (ICSC)

12.7.9 Skin Prevention

Protective clothing. Protective gloves.

- ILO International Chemical Safety Cards (ICSC)

12.7.10 Eye Prevention

Wear safety goggles, face shield or eye protection in combination with breathing protection.

- ILO International Chemical Safety Cards (ICSC)

12.7.11 Ingestion Prevention

Do not eat, drink, or smoke during work.

- ILO International Chemical Safety Cards (ICSC)

12.8 Stability and Reactivity

12.8.1 Air and Water Reactions

Insoluble in water.

- CAMEO Chemicals

12.8.2 Reactive Group

Phenols and Cresols

- CAMEO Chemicals

12.8.3 Reactivity Profile

2,4-DIMETHYLPHENOL is a very weak acid (pKa = 10.6) (NTP, 1992). Incompatible with acid chlorides, acid anhydrides, bases and oxidizing agents. Corrodes steel, brass, copper and copper alloys (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

12.9 Transport Information

12.9.1 DOT Emergency Guidelines

/GUIDE 153: SUBSTANCES - TOXIC AND/OR CORROSIVE (COMBUSTIBLE)/ Health: TOXIC; inhalation, ingestion, or skin contact with material may cause severe injury or death. Contact with molten substance may cause severe burns to skin and eyes. Avoid any skin contact. Effects of contact or inhalation may be delayed. Fire may produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause pollution. /Xylenols; Xylenols, liquid; Xylenols, solid/

U.S. Department of Transportation. 2004 Emergency Response Guidebook. A Guide book for First Responders During the Initial Phase of a Dangerous Goods/Hazardous Materials Incident. Washington, D.C. 2004

- Hazardous Substances Data Bank (HSDB)

/GUIDE 153: SUBSTANCES - TOXIC AND/OR CORROSIVE (COMBUSTIBLE)/ Fire or Explosion: Combustible material: may burn but does not ignite readily. When heated, vapors may form explosive mixtures with air: indoors, outdoors, and sewers explosion hazards. Those substances designated with a "P" may polymerize explosively when heated or involved in a fire. Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated. Runoff may pollute waterways. Substance may be transported in a molten form. /Xylenols; Xylenols, liquid; Xylenols, solid/

U.S. Department of Transportation. 2004 Emergency Response Guidebook. A Guide book for First Responders During the Initial Phase of a Dangerous Goods/Hazardous Materials Incident. Washington, D.C. 2004

- Hazardous Substances Data Bank (HSDB)

/GUIDE 153: SUBSTANCES - TOXIC AND/OR CORROSIVE (COMBUSTIBLE)/ Public Safety: CALL Emergency Response Telephone Number ... . 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. Keep unauthorized personnel away. Stay upwind. Keep out of low areas. Ventilate enclosed areas. /Xylenols; Xylenols, liquid; Xylenols, solid/

U.S. Department of Transportation. 2004 Emergency Response Guidebook. A Guide book for First Responders During the Initial Phase of a Dangerous Goods/Hazardous Materials Incident. Washington, D.C. 2004

▸ Hazardous Substances Data Bank (HSDB)

/GUIDE 153: SUBSTANCES - TOXIC AND/OR CORROSIVE (COMBUSTIBLE)/ Protective Clothing: Wear positive pressure self-contained breathing apparatus (SCBA). Wear chemical protective clothing that is specifically recommended by the manufacturer. It may provide little or no thermal protection. Structural firefighters' protective clothing provides limited protection in fire situations ONLY; it is not effective in spill situations where direct contact with the substance is possible. /Xylenols; Xylenols, liquid; Xylenols, solid/

U.S. Department of Transportation. 2004 Emergency Response Guidebook. A Guide book for First Responders During the Initial Phase of a Dangerous Goods/Hazardous Materials Incident. Washington, D.C. 2004

▸ Hazardous Substances Data Bank (HSDB)

For more DOT Emergency Guidelines (Complete) data for 2,4-DIMETHYLPHENOL (8 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

12.9.2 Shipping Name/ Number DOT/UN/NA/IMO

UN 2261; Dimethylphenols

▸ Hazardous Substances Data Bank (HSDB)

IMO 6.1; Dimethylphenols

▸ Hazardous Substances Data Bank (HSDB)

12.9.3 Shipment Methods and Regulations

No person may /transport,/ offer or accept a hazardous material for transportation in commerce unless that person is registered in conformance ... and the hazardous material is properly classed, described, packaged, marked, labeled, and in condition for shipment as required or authorized by ... /the hazardous materials regulations (49 CFR 171-177)./

49 CFR 171.2 (7/1/96)

▸ Hazardous Substances Data Bank (HSDB)

The International Air Transport Association (IATA) Dangerous Goods Regulations are published by the IATA Dangerous Goods Board pursuant to IATA Resolutions 618 and 619 and constitute a manual of industry carrier regulations to be followed by all IATA Member airlines when transporting hazardous materials.

IATA. Dangerous Goods Regulations. 38th ed. Montreal, Canada and Geneva, Switzerland: International Air Transport Association, Dangerous Goods Board, January, 1997., p. 230

▸ Hazardous Substances Data Bank (HSDB)

The International Maritime Dangerous Goods Code lays down basic principles for transporting hazardous chemicals. Detailed recommendations for individual substances and a number of recommendations for good practice are included in the classes dealing with such substances. A general index of technical names has also been compiled. This index should always be consulted when attempting to locate the appropriate procedures to be used when shipping any substance or article.

IMDG; International Maritime Dangerous Goods Code; International Maritime Organization p.6248 (1988)

▸ Hazardous Substances Data Bank (HSDB)

12.9.4 DOT Label

Poison

▸ CAMEO Chemicals

12.9.5 Packaging and Labelling

Do not transport with food and feedstuffs. Marine pollutant.

▸ ILO International Chemical Safety Cards (ICSC)

12.9.6 EC Classification

Symbol: T, N; R: 24/25-34-51/53; S: (1/2)-26-36/37/39-45-61; Note: C

- ILO International Chemical Safety Cards (ICSC)

12.9.7 UN Classification

UN Hazard Class: 6.1; UN Pack Group: II

- ILO International Chemical Safety Cards (ICSC)

12.10 Regulatory Information

12.10.1 State Drinking Water Guidelines

(CA) CALIFORNIA 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 400 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)

(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)

12.10.2 Clean Water Act Requirements

Toxic pollutant designated pursuant to section 307(a)(1) of the Clean Water Act and is subject to effluent limitations.

40 CFR 401.15 (7/1/88)

- Hazardous Substances Data Bank (HSDB)

Sufficient data are not available for 2,4-dimethylphenol to derive a level which would protect against the potential toxicity of this compound. Using available organoleptic data, for controlling undesirable taste and odor quality of ambient water, the estimated level for 2,4-dimethylphenol is 400 ug/l. It should be recognized that organoleptic data as a basis for establishing a water quality criterion have limitations and have no demonstrated relationship to potential adverse human health effects.

USEPA; Ambient Water Quality Criteria Doc: 2,4-Dimethylphenol p.vi (1980) EPA 440/5-80-0269

- Hazardous Substances Data Bank (HSDB)

12.10.3 CERCLA Reportable Quantities

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; In the Washington D.C. metropolitan area (202) 426-2675. The rule for determining when notification is required is stated in 40 CFR 302.4 (section IV. D.3.b).

40 CFR 302.4 (7/1/97)

- Hazardous Substances Data Bank (HSDB)

12.10.4 RCRA Requirements

U101; As stipulated in 40 CFR 261.33, when 2,4-dimethylphenol, as a commercial chemical product or manufacturing chemical intermediate or an off-specification commercial chemical product or a manufacturing chemical intermediate, becomes a waste, it must be managed according to Federal and/or State hazardous waste regulations. Also defined as a hazardous waste is any residue, contaminated soil, water, or other debris resulting from the cleanup of a spill, into water or on dry land, of this waste. Generators of small quantities of this waste may qualify for partial exclusion from hazardous waste regulations (40 CFR 261.5).

40 CFR 261.33 (7/1/97)

- Hazardous Substances Data Bank (HSDB)

12.11 Other Safety Information

12.11.1 Special Reports

USEPA; Ambient Water Quality Criteria Doc: 2,4 Dimethylphenol (1980) EPA 440/5-80-044.

▸ Hazardous Substances Data Bank (HSDB)

Toxikologische Bewertung. 137 (1995). Summary and assessment of 2,4-xylenol.

▸ Hazardous Substances Data Bank (HSDB)

EPA. EPA/600/8-88/031 p.30 (1987). Health effects assessment for dimethylphenols.

▸ Hazardous Substances Data Bank (HSDB)

Tucker JD et al; Mutat Res 297 (2): 101-80 (1993). Sister-chromatid exchange: second report of the Gene-Tox Program.

▸ Hazardous Substances Data Bank (HSDB)

13 Toxicity

13.1 Toxicological Information

13.1.1 NIOSH Toxicity Data

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

13.1.2 Exposure Routes

The substance can be absorbed into the body by inhalation, by ingestion and through the skin.

- ILO International Chemical Safety Cards (ICSC)

13.1.3 Inhalation Symptoms

Burning sensation. Cough. Sore throat. Shortness of breath.

- ILO International Chemical Safety Cards (ICSC)

13.1.4 Skin Symptoms

Redness. Pain. Skin burns.

- ILO International Chemical Safety Cards (ICSC)

13.1.5 Eye Symptoms

Redness. Pain. Severe burns.

- ILO International Chemical Safety Cards (ICSC)

13.1.6 Ingestion Symptoms

Burning sensation. Abdominal pain. Nausea. Vomiting. Shock or collapse.

- ILO International Chemical Safety Cards (ICSC)

13.1.7 Acute Effects

- ChemIDplus

13.1.8 Interactions

A SPONTANEOUSLY DEVELOPING VASOCONSTRICTION IN ISOLATED PERFUSED LUNG AND THE VASOCONSTRICTION CAUSED BY ARTERIALLY INJECTED ATP 50 UG WERE BOTH INHIBITED BY THE ADDITION TO THE PERFUSATE OF VARIOUS PHENOLS INCLUDING 2,4-XYLENOL.

PMID:5659747
LUNDE PK M ET AL; ACTA PHYSIOL SCAND 72 (3): 331-7 (1968)

- Hazardous Substances Data Bank (HSDB)

13.1.9 Antidote and Emergency Treatment

Basic treatment: Establish a patent airway. 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 ... . Anticipate seizures and treat if necessary ... . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport ... . Administer activated charcoal ... . Dilution may be contraindicated because it may increase absorption. Do not use emetics ... . Cover skin burns with dry sterile dressings after decontamination ... . /Phenols and Related compounds/

Bronstein, A.C., P.L. Currance; Emergency Care for Hazardous Materials Exposure. 2nd ed. St. Louis, MO. Mosby Lifeline. 1994., p. 243-4

- 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 respiratory arrest. Positive-pressure ventilation techniques with a bag-valve-mask device may be beneficial. Monitor cardiac rhythm and treat arrhythmias if necessary ... . Start an IV with D5W TKO /SRP: "To keep open", minimal flow rate/. Use lactated Ringer's if signs of hypovolemia are present. Watch for signs of fluid overload. Consider drug therapy for pulmonary edema ... . For hypotension with signs of hypovolemia, administer fluid cautiously. Consider vasopressors for hypotension with a normal fluid volume. Watch for signs of fluid overload ... . Administer 1% solution methylene blue if patient is symptomatic with severe hypoxia, cyanosis, and cardiac compromise not responding to oxygen. ... . Treat seizures with diazepam (Valium) ... . Use proparacaine hydrochloride to assist eye irrigation ... . /Phenols and Related Compounds/

Bronstein, A.C., P.L. Currance; Emergency Care for Hazardous Materials Exposure. 2nd ed. St. Louis, MO. Mosby Lifeline. 1994., p. 139

- Hazardous Substances Data Bank (HSDB)

13.1.10 Human Toxicity Excerpts

The trichlorophenols and 2,4-dimethylphenol may be carcinogens.

Dreisbach, R.H. Handbook of Poisoning. 12th ed. Norwalk, CT: Appleton and Lange, 1987., p. 366

- Hazardous Substances Data Bank (HSDB)

2,4-Dimethylphenol appears to be a topical cocarcinogen, but its role as a primary cancer-producing agent is uncertain.

Sittig, M. Handbook of Toxic and Hazardous Chemicals and Carcinogens, 1985. 2nd ed. Park Ridge, NJ: Noyes Data Corporation, 1985., p. 368

- Hazardous Substances Data Bank (HSDB)

Lysol poisoning has been associated with incomplete abortions, shock, tachycardia, leukocytosis, hemolysis, fever, central nervous system irritability, respiratory ... /insufficiency/ associated with pulmonary edema and/or oil emboli, local tissue necrosis with uterine hemorrhage, and anemia.

Ellenhorn, M.J., S. Schonwald, G. Ordog, J. Wasserberger. Ellenhorn's Medical Toxicology: Diagnosis and Treatment of Human Poisoning. 2nd ed. Baltimore, MD: Williams and Wilkins, 1997., p. 1211

▸ Hazardous Substances Data Bank (HSDB)

The low-molecular-weight phenols 2-methylol phenol, 4-methylol phenol, 2,4,6-trimethylol phenol, 3-methylol phenol, 2,4-dimethylol phenol, and 2,6-dimethylol phenol are contact sensitizers in resins based on phenol and formaldehyde. ... In patients hypersensitive to resins based on phenol and formaldehyde and methylphenol, it is for diagnostic, therapeutic and preventive reasons necessary to know their cross-reaction patterns, which this study was therefore designed to investigate. In patients with contact allergy to a resin based on phenol and formaldehyde and at least 1 methylphenol, additional patch testing was performed with 6 methylphenol and 13 chemically related compounds. The 19 substances were tested at equimolar concentrations and in serial dilutions. Investigations by high-performance liquid chromatography were carried out to exclude contamination as the cause of the patch test reactions. Probable cross-reacting substances were o-cresol, p-cresol, salicylaldehyde, 2,4-dimethylphenol, and 2,6-dimethylphenol.

PMID:9285170

Bruze M, Zimerson E; Contact Dermatitis 37 (2): 82-6 (1997)

▸ Hazardous Substances Data Bank (HSDB)

Moderately toxic by ingestion and skin contact.

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 3405

▸ Hazardous Substances Data Bank (HSDB)

13.1.11 Non-Human Toxicity Excerpts

Smokehouse smoke, which is used for flavoring meat products, was investigated for its mutagenic activity in the Salmonella typhimurium assay. Fractions free of polycyclic aromatic hydrocarbons but containing phenol compounds were the chief concern. One of the most abundantly occurring phenol compounds, 2,4-dimethylphenol, gave negative results when it was tested for mutagenicity at 5 concentrations up to 5,000 ug/plate, with and without S-9 mix, using five strains of Salmonella typhimurium.

PMID:6751955

Pool BL, Lin PZ; Food Chem Toxicol 20 (4): 383-92 (1982)

▸ Hazardous Substances Data Bank (HSDB)

Chinese hamster ovary, rabbit alveolar macrophage, Syrian hamster embryo, BALB/3T3 mouse, and human neonatal fibroblast cells were employed in a statistical evaluation of the relative sensitivity of the cells to toxic substances. The cells were exposed to 2,4-dimethylphenol (40 ug/ml). A filter disk technique was used to measure the inhibition of protein and DNA synthesis. Relative sensitivity of cells to 2,4-dimethylphenol based on inhibition of protein synthesis: Syrian hamster embryo cells most sensitive followed by BALB/3T3 and Chinese hamster ovary cells; human neonatal fibroblast cells and rabbit alveolar macrophage cells equivalent. Based on DNA synthesis: Syrian hamster embryo cells, BALB/3T3 cells, human neonatal fibroblast cells, and Chinese hamster ovary cells were equivalent.

PMID:6685623

Garrett NE et al; Environ Res 32 (2): 466-73 (1983)

▸ Hazardous Substances Data Bank (HSDB)

Embryos of fathead minnows were more resistant to 2,4-dimethylphenol than were larval or juvenile life stages. Growth of 28 day old fish was the most sensitive indicator of stress during exposures to 2,4-dimethylphenol. Based on these effects, the established maximum acceptable toxicant concentration for fathead minnows in Lake Superior water lies between 1,970 and 3,110 ug/l for 2,4-dimethylphenol.

PMID:7073320

Holcombe GW et al; Arch Environ Contam Toxicol 11 (1): 73-8 (1982)

▸ Hazardous Substances Data Bank (HSDB)

Fathead minnows lost schooling behavior, were hyperactive, had hemorrhaging, and lost equilibrium prior to death.

Geiger D.L., Poirier S.H., Brooke L.T., Call D.J., (eds). Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales Promelas). Vol. II. Superior, Wisconsin: University of Wisconsin-Superior, 1985., p. 185

▸ Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Excerpts (Complete) data for 2,4-DIMETHYLPHENOL (16 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

13.1.12 Non-Human Toxicity Values

LD50 Rat dermal 1040 mg/kg

USEPA; Ambient Water Quality Criteria Doc: 2,4-Dimethylphenol p.C-12 (1980) EPA 440/5-80-044

▸ Hazardous Substances Data Bank (HSDB)

LD50 MOUSE IP 150 MG/KG

National Research Council. Drinking Water & Health Volume 1. Washington, DC: National Academy Press, 1977., p. 730

▸ Hazardous Substances Data Bank (HSDB)

LD50 Rat oral 2300 mg/kg

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 3405

▸ Hazardous Substances Data Bank (HSDB)

LD50 Mouse oral 809 mg/kg

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 3405

▸ Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Values (Complete) data for 2,4-DIMETHYLPHENOL (6 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

13.1.13 Ecotoxicity Values

LC50 Pimephales promelas (fathead minnow) 17 mg/l/96 hr /Flow through bioassay/

PMID:7260426
Phipps GL et al; Bull Environ Contam Toxicol 26 (5): 585-93 (1981)

▸ Hazardous Substances Data Bank (HSDB)

TLm Carassius carassius (crucian carp) 30 mg/l/24 hr /Conditions of bioassay not specified/

Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983., p. 1196

▸ Hazardous Substances Data Bank (HSDB)

LC50 Pimephales promelas (fathead minnow) 16.6 mg/l/96 hr (confidence limit 16.1-17.1 mg/l) at 25.6 °C (hardness 45.7 mg/l CaCO3, pH 8.25) /Conditions of bioassay not specified/

Geiger D.L., Poirier S.H., Brooke L.T., Call D.J., (eds). Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales Promelas). Vol. II. Superior, Wisconsin: University of Wisconsin-Superior, 1985., p. 186

▸ Hazardous Substances Data Bank (HSDB)

LC50 Pimephales promelas (fathead minnow) 13,650 ug/l/192 hr /Static, unmeasured bioassay/

USEPA; Ambient Water Quality Criteria Doc: 2,4-Dimethylphenol p.B-1 (1980) EPA 440/5-80-0269

▸ Hazardous Substances Data Bank (HSDB)

For more Ecotoxicity Values (Complete) data for 2,4-DIMETHYLPHENOL (9 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

13.2 Ecological Information

13.2.1 US EPA Regional Screening Levels for Chemical Contaminants

Resident Soil (mg/kg)	1.30e+02
Industrial Soil (mg/kg)	1.60e+03
Tapwater (ug/L)	3.60e+01
Risk-based SSL (mg/kg)	4.20e-02
Chronic Oral Reference Dose (mg/kg-day)	2.00e-02
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

13.2.2 US EPA Regional Removal Management Levels for Chemical Contaminants

Resident Soil (mg/kg)	3.80e+03
Industrial Soil (mg/kg)	4.90e+04
Tapwater (ug/L)	1.10e+03
Chronic Oral Reference Dose (mg/kg-day)	2.00e-02
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

13.2.3 ICSC Environmental Data

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

▸ ILO International Chemical Safety Cards (ICSC)

13.2.4 Environmental Fate/Exposure Summary

2,4-Dimethylphenol's production and use for the preparation of coal tar disinfectants, in the manufacture of artificial resins, as a constituent of coal tar creosote, and as a component of gasoline, rubber, and automobile and diesel exhaust may result in its release to the environment through various waste streams. 2,4-Dimethylphenol has been found to occur naturally in tobacco and marijuana smoke and in black tea. If released to air, a vapor pressure of 0.102 mm Hg at 25 °C indicates that 2,4-dimethylphenol will exist solely as a vapor in the ambient atmosphere. Vapor-phase 2,4-dimethylphenol 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 5.3 hours. There is potential for the direct photolysis of 2,4-dimethylphenol since its absorption band extends over 290 nm and thus 2,4-dimethylphenol may absorb light in the environmental UV spectrum. If released to soil, 2,4-dimethylphenol is expected to have moderate mobility based upon an estimated Koc of 430. Volatilization from moist soil surfaces is expected to be an important fate process based upon a Henry's Law constant of 1.7X10-5 atm-cu m/mole. Complete biodegradation of 2,4-dimethylphenol has occurred in 4 days within a hard, carbonaceous woody loam. The biodegradation half-life of 2,4-dimethylphenol from Texas soil and Mississippi soil was determined to be 1.5 and 3.5 days, respectively. If released into water, 2,4-dimethylphenol is expected to adsorb very little to suspended solids and sediment in the water column based upon the estimated Koc. 95% biodegradation was obtained for 2,4-dimethylphenol in a screening test with an adapted activated sludge seed after 5 days. In addition, it has been reported that 2,4-dimethylphenol was readily degraded in St. Lawrence River water. Biodegradation under anaerobic conditions failed to occur in one study and 48% degradation occurred after 8 weeks in another study. Volatilization from water surfaces is expected to be an important fate process based upon this compound's Henry's Law constant. Estimated volatilization half-lives for a model river and model lake are 3 days and 22 days, respectively. A BCF of 150 in bluegill sunfish suggests the potential for bioconcentration in aquatic organisms is moderate. Hydrolysis is not expected to occur due to the lack of hydrolyzable functional groups. Occupational exposure to 2,4-dimethylphenol may occur through inhalation of this compound at workplaces where 2,4-dimethylphenol is produced or used. The general population may be exposed to 2,4-dimethylphenol via inhalation of ambient air (i.e., tobacco smoke and automobile exhaust), ingestion of food (fish), and contact with other products containing 2,4-dimethylphenol. (SRC)

▸ Hazardous Substances Data Bank (HSDB)

13.2.5 Natural Pollution Sources

2,4-Dimethylphenol is a constituent of coal(1) and has been found in tobacco and marijuana mainstream smoke(2,3), and in black tea(4).

(1) Verschueren K; Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York, NY: Van Nostrand Reinhold (1996) (2) Hoffman D et al; Rec Adv Phytochem 9: 63-81 (1975) (3) Baggett MS, Morie GP; Tobacco Sci 17: 37-40 (1973) (4) Kaiser HE; Cancer 20: 614-6 (1966)

▸ Hazardous Substances Data Bank (HSDB)

13.2.6 Artificial Pollution Sources

/SRP/: DIMETHYLPHENOLS OCCUR IN SHALE OIL PROCESS WATER, INDUSTRIAL WASTE WATER, AIRBORNE PARTICULATES, ... AND EVOLUTES FROM WASTE CHEMICAL DUMPS. /DIMETHYLPHENOLS/

▸ Hazardous Substances Data Bank (HSDB)

The nature and extent of pollution was determined at the site of a former pine tar manufacturer in Gainsville, Florida. In 1979 the EPA conducted an investigation of this area. Compound distribution at various areas about the site revealed that, in addition to groundwater leaching of soluble phenolics, insoluble contaminants were spread by a dike-breach incident and subsequent construction activities. Differences in the patterns of chemicals in various wells suggested that more than one source of pollution occurred. The distribution of compounds about the site indicated that a general clean-up would not be cost-effective. Placement of an intereceptor to collect groundwater seepage that contaminated surface water was considered as an alternative. One of the 43 compounds identified in soil extracts was 2,4-dimethylphenol.

McCreary JJ et al; Chemosphere 12 (11-12): 1619-32 (1983)

▸ Hazardous Substances Data Bank (HSDB)

2,4-Dimethylphenol's use for the preparation of coal tar disinfectants (1), in the manufacture of artificial resins(1), as a constituent of coal tar creosote (0.5 wt%)(2), as a raw material for antioxidants for gasoline and rubber(3), and as a component of automobile and diesel exhaust(4,5) may result in its release to the environment through various waste streams(SRC). In addition, 2,4-dimethylphenol may also be released in asphalt and roadway runoff, washing of dyed materials, and general use of pharmaceuticals, fuels, plastic, and pesticides(2). Dimethylphenols, of which 2,4-dimethylphenol is an isomer, are components of disinfectants, solvents, insecticides, fungicides, plasticizers, rubber chemicals, additives to lubricants and gasolines, wetting agents and dyestuffs(9).

(1) Budavari S et al; The Merck Index: an Encyclopedia of Chemicals And Drugs. 12th Ed. Whitehouse Station,NJ: Merck And Co, Inc (1996) (2) Verschueren K; Handbook of Environmental Data on Organic Chemicals. 3rd ed. NY,NY: Van Nostrand Reinhold (1996) (3) Fiege H; Ullmann's Encycl Indust Chem. 5th ed. Deerfield Beach,FL: VCH Pub A8: 25-59 (1987) (4) Hampton CV et al; Environ Sci Technol 16: 287-98 (1982) (5) Graedel TE et al; Atmospheric Chemical Compounds. London,UK: Academic Press p. 250 (1986) (9) Lewis RJ; Hawley's Condensed Chemical Dictionary. 12th Ed. NY,NY: Van Nostrand Reinhold Company (1993)

▸ **Hazardous Substances Data Bank (HSDB)**

13.2.7 Environmental Fate

TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 430(SRC), determined from a log Kow of 2.30(2) and a regression-derived equation(3), indicates that 2,4-dimethylphenol is expected to have moderate mobility in soil(SRC). Volatilization of 2,4-dimethylphenol from moist soil surfaces is expected to be an important fate process(SRC) given a Henry's Law constant of 1.7X10-5 atm-cu m/mole (4). 2,4-Dimethylphenol is not expected to volatilize from dry soil surfaces(3) based upon a vapor pressure of 0.102 mm Hg at 25 °C(5). 2,4-Dimethylphenol has been reported to completely biodegrade from soil in 4 days at a temperature of 19 °C(6) and the biodegradation half-life of 2,4-dimethylphenol from Texas soil and Mississippi soil was determined to be 1.5 and 3.5 days, respectively(7).

(1) Swann RL et al; Res Rev 85: 23 (1983) (2) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, And Steric Constants. ACS Prof Ref Book. Washington,DC: Amer Chem Soc (1995) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington,DC: Amer Chem Soc pp. 4-9 (1990) (4) Smith JR et al; Water Environ Res 65: 804-18 (1993) (5) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation. Design Inst Phys Prop Data, Amer Inst Chem Eng NY,NY: Hemisphere Pub Corp 5 Vol (1993) (6) Medvedev V, Davidov VD; pp. 245-54 in Decomposition of Toxic and Nontoxic Organic Compounds in Soil. Overcash MR ed. Ann Arbor,MI: Ann Arbor Sci Publ (1981) (7) Loehr RC; Treatability Potential for EPA Listed Hazardous Wastes in Soil. USEPA/600/2-89/011. USEPA. Robert S Kerr Environ Res Lab, Ada, OK pp. 1-118 (1989)

▸ **Hazardous Substances Data Bank (HSDB)**

AQUATIC FATE: Based on a classification scheme(1), a Koc value of 430(SRC), determined from a log Kow of 2.30(2) and a regression-derived equation(3), indicates that 2,4-dimethylphenol is expected to adsorb very little to suspended solids and sediment in water(SRC). 2,4-Dimethylphenol is expected to volatilize from water surfaces(3,SRC) based upon a Henry's Law constant of 1.7X10-5 atm-cu m/mole(4). Estimated volatilization half-lives for a model river and model lake are 3 days and 22 days, respectively(3,SRC). According to a classification scheme(5), a BCF of 150 in bluegill sunfish(6) suggests bioconcentration in aquatic organisms is moderate(SRC). In humic waters, degradation by the reaction with peroxy radicals should ensue with a half-life on the order of hours(7). 2,4-Dimethylphenol is not expected to undergo hydrolysis in the environment due to the lack of hydrolyzable functional groups(3). Screening studies indicate that 95% removal of 2,4-dimethylphenol was obtained after 5 days using an activated sludge inoculum(8). In addition, it has been reported that 2,4-dimethylphenol was readily degraded in St. Lawrence River water(9). Methanogenic consortia failed to anaerobically biodegrade 2,4-dimethylphenol after 24 days in one study(10); in two standardized anaerobic bioassays using a digester sludge, 2,4-dimethylphenol yielded no more than 10% of theoretical methane(11).

(1) Swann RL et al; Res Rev 85: 23 (1983) (2) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, And Steric Constants. ACS Prof Ref Book. Washington,DC: Amer Chem Soc (1995) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington,DC: Amer Chem Soc pp. 4-9, 5-4, 5-10, 7-4, 7-5, 15-1 to 15-29 (1990) (4) Smith JR et al; Water Environ Res 65: 804-18 (1993) (5) Franke C et al; Chemosphere 29: 1501-14 (1994) (6) Veith GD et al; pp. 116-29 in ASTM STP 707. Aquatic Toxicology. Easton JG et al, eds. Amer Soc Test Mater (1980) (7) Mill T; Environ Toxicol Chem 1: 135-41 (1982) (8) Pitter P; Water Res 10: 231-5 (1976) (9) Visser SA et al; Arch Environ Contam Toxicol 6: 455-70 (1977) (10) Kaminski U et al; J Basic Microbiol 259-65 (1990) (11) Young LY; Toxic Organic Chemicals in Waste Streams NTIS/DE86009 496. DOE/CE/40657-1 Washington,DC: Dept Energy p. 92 (1986)

▸ **Hazardous Substances Data Bank (HSDB)**

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), 2,4-dimethylphenol, which has a vapor pressure of 0.102 mm Hg at 25 °C(2), is expected to exist solely as a vapor in the ambient atmosphere. Vapor-phase 2,4-dimethylphenol 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 5.3 hours(SRC) from its rate constant of 7.20X10-11 cu cm/molecule-sec at 25 °C(3). 2,4-Dimethylphenol has an absorption band at 296 nm (maximum) and extends over 320 nm, thus making it a candidate for direct photochemical degradation(5,6). Night-time degradation in urban areas should occur rapidly through reaction with atmospheric nitrate radicals, as rate constants for this reaction with phenolic compounds are approximately 250 times faster than with hydroxyl radicals(7,SRC).

(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation. Design Inst Phys Prop Data, Amer Inst Chem Eng NY,NY: Hemisphere Pub Corp 5 Vol (1993) (3) Atkinson R; J Phys Chem Ref Data. Monograph 2 (1994) (5) Callahan MA et al; Water-Related Environ Fate of 129 Priority Pollut Vol.II USEPA-440/4-79-029B (1979) (6) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington,DC: Amer Chem Soc pp. 7-4, 7-5 (1990) (7) Carter WPL et al; Environ Sci Tech 15: 829-31 (1981)

▸ **Hazardous Substances Data Bank (HSDB)**

13.2.8 Environmental Biodegradation

... A series of experiments /were carried out/ ... to duplicate the conditions for biodegradability that would occur in a river that was receiving phenolic waste effluents from a coking plant. Unsubstituted phenol decomposed rapidly, cresols exhibited a lag period of several days, but 2,4- and 2,3- dimethylphenol seemed to be very persistent.

Callahan, M.A., M.W. Slimak, N.W. Gabel, et al. Water-Related Environmental Fate of 129 Priority Pollutants. Volume II. EPA-440/4-79-029b. Washington, D.C.: U.S. Environmental Protection Agency, December 1979., p. 91-5

▸ **Hazardous Substances Data Bank (HSDB)**

In shake flask studies, an initial 2,4-dimethylphenol concentration of 0.2 ug/ml was reduced to below detection following 2 weeks incubation in contaminated groundwater from the American Creosote Works Superfund site, Pensacola, FL(1). 2,4-Dimethylphenol was readily degraded in St. Lawrence River water(2). The biodegradation half-life of 2,4-dimethylphenol from Texas soil and Mississippi soil was determined to be 1.5 and 3.5 days, respectively(3). Using bacteria isolated from the subsurface of a manufactured gas plant in England, 2,4-dimethylphenol degraded very slowly in contaminated soil; the final decrease in concentration varied from 15-18% of the starting concentration of 165.6 mg/l and a first-order half-life was estimated to be 248 days(4). 2,4-Dimethylphenol degraded in 4 days within a hard, carbonaceous woody loam at 19 °C(5).

(1) Mueller JG et al; Appl Environ Microbiol 57: 1277-285 (1991) (2) Visser SA et al; Arch Environ Contam Toxicol 6: 455-70 (1977) (3) Loehr RC; Treatability Potential for EPA Listed Hazardous Wastes in Soil. USEPA/600/2-89/011. USEPA. Robert S Kerr Environ Res Lab, Ada, OK pp. 1-118 (1989) (4) Thomas AO, Lester JN; Haz Waste Haz Mat 10: 413-30 (1993) (5) Medvedev V, Davidov VD; pp. 245-54 in Decomposition of Toxic and Nontoxic Organic Compounds in Soil. Overcash MR ed. Ann Arbor,MI: Ann Arbor Sci Publ (1981)

▸ **Hazardous Substances Data Bank (HSDB)**

Using a biological treatment simulator, 42.8% theoretical oxygen demand after 10 days was obtained for 2,4-dimethylphenol from a coal gasification waste water feed and an acclimated sludge inoculum(1). 2,4-Dimethylphenol proved to be easily degradable, although at high initial concns, products of 2,4-dimethylphenol biodegradation were inhibitory to biomass growth(2). 2,4-Dimethylphenol, at an initial concn of 100 and 160 mg/cu dm, was shown to be completely degraded in fifteen days using an activated sludge seed(3). 95% removal of 2,4-dimethylphenol in 5 days was achieved in screening studies using activated sludge(4) and 100% degradation occurred in 7 days with a sewage seed(5).

(1) Snider EH, Manning FS; Environ Int 7: 237-58 (1982) (2) Brown SC et al; Wat Res 24: 853-61 (1990) (3) Grossman A, Kusznik W; Environ Protection Engineering 1: 151-62 (1975) (4) Pitter P; Water Res 10: 231-5 (1976) (5) Tabak HH et al; J Water Pollut Contr Fed 53: 1503-18 (1981)

▸ Hazardous Substances Data Bank (HSDB)

ANAEROBIC: It was determined that methanogenic consortia, using Saale river sediment as the inoculum, failed to biodegrade 2,4-dimethylphenol after 24 days(1). An anaerobic gas production test of sewage sludge, a freshwater swamp sediment and a marine sediment was conducted; results revealed 0 to 30% mineralization of 2,4-dimethylphenol in digested sewage sludge and freshwater swamp sediment after an incubation period of 56 days and 0 to 30% mineralization in marine sediment after an incubation period of 96 days(2). In another study, 2,4-dimethylphenol, at an initial concn of 1.22 mg/l, underwent 48% degradation when incubated in coal tar-contaminated groundwater in an anaerobic digester for 8 weeks(3). Using a 10% v/v municipal digester sludge, 20-200 mg/l 2,4-dimethylphenol yielded no more than 10% of theoretical methane in two standardized anaerobic bioassays(4).

(1) Kaminski U et al; J Basic Microbiol 30: 259-65 (1990) (2) Madsen T et al; Chemosphere 31: 4243-58 (1995) (3) Godsy EM et al; Bull Environ Contam Toxicol 30: 261-68 (1983) (4) Young LY; Toxic Organic Chemicals in Waste Streams NTIS/DE86009 496. DOE/CE/40657-1 Washington,DC: Dept Energy p. 92 (1986)

▸ Hazardous Substances Data Bank (HSDB)

13.2.9 Environmental Abiotic Degradation

The rate constant for the vapor-phase reaction of 2,4-dimethylphenol with photochemically-produced hydroxyl radicals has been determined to be 7.20X10-11 cu cm/molecule-sec at 25 °C(1). This corresponds to an atmospheric half-life of about 5.3 hours at an atmospheric concn of 5X10+5 hydroxyl radicals per cu cm(1). 2,4-Dimethylphenol has an absorption band at 296 nm (maxima) which extends over 320 nm, thus making it a candidate for direct photochemical degradation(2,3). Night-time degradation in urban areas should occur rapidly through reaction with atmospheric nitrate radicals, as rate constants for this reaction with phenolic compounds are approximately 250 times faster than with hydroxyl radicals(4,SRC). Peroxy radicals found in humic waters react with phenols; the half-lives can be measured in hours(5). 2,4-Dimethylphenol is not expected to undergo hydrolysis in the environment due to the lack of hydrolyzable functional groups(3).

(1) Atkinson R; J Phys Chem Ref Data. Monograph 2 (1994) (2) Callahan MA et al; Water-Related Environ Fate of 129 Priority Pollut Vol.II USEPA-440/4-79-029B (1979) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington,DC: Amer Chem Soc pp. 7-4, 7-5 (1990) (4) Carter WPL et al; Environ Sci Tech 15: 829-31 (1981) (5) Mill T; Environ Toxicol Chem 1: 135-41 (1982)

▸ Hazardous Substances Data Bank (HSDB)

13.2.10 Environmental Bioconcentration

A BCF of 150 was determined for 2,4-dimethylphenol in bluegill sunfish and 28 days exposure(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is high.

(1) Veith GD et al; ASTM STP 707. Aquatic Toxicology. Easton JG et al, eds. Amer Soc Test Mater pp. 116-29 (1980) (2) Franke C et al; Chemosphere 29: 1501-14 (1994)

▸ Hazardous Substances Data Bank (HSDB)

13.2.11 Soil Adsorption/Mobility

The Koc of 2,4-dimethylphenol is estimated as 430(SRC), using a log Kow of 2.30(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 2,4-dimethylphenol is expected to have moderate mobility in soil(SRC). The estimated Koc for 2,4-dimethylphenol is consistent with the Koc in river sediment and coal sediment from a pond near Leipzig, Germany which was determined to be 120 and 105 (log Koc = 2.08 and 2.02), respectively(4).

(1) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, And Steric Constants. ACS Prof Ref Book. Washington,DC: American Chemical Society (1995) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington,DC: Amer Chem Soc pp. 4-9 (1990) (3) Swann RL et al; Res Rev 85: 23 (1983) (4) Kopinke FD et al; Environ Sci Technol 29: 941-50 (1995)

▸ Hazardous Substances Data Bank (HSDB)

13.2.12 Volatilization from Water/Soil

The Henry's Law constant for 2,4-dimethylphenol is 1.7X10-5 atm-cu m/mole(1). This Henry's Law constant indicates that 2,4-dimethylphenol 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)(3) is estimated as 3 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 approximately 22 days(SRC). 2,4-Dimethylphenol's Henry's Law constant(1,2) indicates that volatilization from moist soil surfaces is expected to occur(SRC). 2,4-Dimethylphenol is not expected to volatilize from dry soil surfaces(SRC) based upon a vapor pressure of 0.102 mm Hg(3).

(1) Smith JR et al; Water Environ Res 65: 804-18 (1993) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington,DC: Amer Chem Soc pp. 15-1 to 15-29 (1990) (3) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation. Design Inst Phys Prop Data, Amer Inst Chem Eng NY,NY: Hemisphere Pub Corp 5 Vol (1993)

▸ Hazardous Substances Data Bank (HSDB)

13.2.13 Environmental Water Concentrations

GROUNDWATER: The concn of 2,4-dimethylphenol in groundwater collected from a wood-preserving plant at Pensacola, FL in 1985 was determined to be 1.33-9.68 mg/l(1). Groundwater samples collected from three creosote- contaminated sites in Denmark, date unspecified, were found to contain 2,4-dimethylphenol ranging in concn from below detection to 2090 ug/l, analyzed with 2,5-dimethylphenol(2). 10 of 11 wells underlying a former pine-tar manufacturing facility in Gainesville, FL were found to contain 2,4-dimethylphenol ranging in concn from 1-9400 ug/l (including 2,5-dimethylphenol)(3). 2,4-Dimethylphenol was detected at a concn of 0.2 mg/l in groundwater near an abandoned wood preservative manufacturing plant in Florida(4). Water samples collected during December 1986 from Gas Works Park, Seattle, WA were found to contain 2,4-dimethylphenol ranging in concn from below detection to 1.0 mg/l(5). Studies near a wood preserving facility in Pensacola, FL detected 2,4-dimethylphenol in ground water at all four sites in a sand aquifer, concns ranging from 0-5.65 mg/l; while detected in samples from 6,12, 18, and 24 m depth, 2,4-dimethylphenol was not detected at 30 m depth(6). 2,4-Dimethylphenol was also identified in the leachate from a sanitary landfill in Barcelona, Spain(7).

(1) Goerlitz DF; pp. 295-355 in Environ Sci Pollut Control Ser 4(Groundwater Contamination and Analysis at Hazardous Waste Sites) (1992) (2) Johansen SS et al; GWMR 17: 106-15 (1997) (3) McCreary JJ et al; Chemosphere 12: 1619-32 (1983) (4) Middaugh DP et al; Arch Environ Contam Toxicol 21: 233-44 (1991) (5) Turney GL, Goerlitz DF; GWMR 10: 187-98 (1990) (6) Goerlitz DF et al; Environ Sci Technol 19: 955-61 (1985) (7) Albaiges J et al; Wat Res 20: 1153-59 (1986)

▸ Hazardous Substances Data Bank (HSDB)

GROUNDWATER: Samples collected on September 9, 1980 from an uncontaminated well bordering a US Army installation site in Bristol, RI revealed that the average concn of 2,4-dimethylphenol was 26 ug/l(1). A study of groundwater contamination at 6 Superfund sites across the U.S. detected 2,4-dimethylphenol in the Biscayne, FL Aquifer study area, concn of 110 ug/l(2). The average concn of 2,4-dimethylphenol in the groundwater near 5 wood treatment facilities sampled in the US was 1,219 ug/l(3). The concn of 2,4-dimethylphenol identified at a closed wood-to-charcoal conversion plant in McKean county, PA in 2 of 3 groundwater wells was estimated as 34 and 360 mg/l(4). At a closed, filled, landfill at Hipps Road landfill, FL, 2,4-dimethylphenol was detected in 1 of 3 groundwater wells at 13 ug/l(5). 2,4-Dimethylphenol was identified in groundwater at a unauthorized disposal site in Pemberton Township, NJ at a concn of 32 ug/l(6).

(1) Beltis K et al; Chemical Analysis Support: Limited Analysis of Bristol, Rhode Island Well Water Samples. US Army Tox Hazard Mat Agency, Aberdeen Proving Ground,MD. Report No. DRXTH-TE-CR-2135, AD-A120-636 (1982) (2) Canter LW, Sabatini DA; Intern J Environ Studies 46: 35-57 (1994) (3) Rosenfeld JK, Plumb RH; Ground Water Environ Rev 11: 133-40 (1991) (4) USEPA; Superfund Record of Decision (EPA Region 3). USEPA/ROD/RO3-86/024 (1987) (5) USEPA; Superfund Record of Decision (EPA Region 4): USEPA/ROD/RO4-86/010 (1986) (6) USEPA; Superfund Record of Decision (EPA Region 2) USEPA/ROD/RO2-86/031. (NTIS PB87-188470) (1987)

▶ Hazardous Substances Data Bank (HSDB)

DRINKING WATER: 2,4-Dimethylphenol was listed as having been identified in drinking water in the USA(1,2) as well as being detected 5 times in finished drinking water samples collected across the United States in 1977(3).

(1) Kopfler FC et al; Human Exposure to Water Pollutants Adv Environ Sci Technol 8 (Fate Pollut Air Water Environ): 419-33 (1977) (2) Shakelford NM, Keith LH; Frequency of Organic Compounds Identified in Water USEPA-600/4-76-062 (1976) (3) Garrison AW et al; in Pergamon Ser Environ Sci 1 (Aquat Pollut: Transform Biol Eff 1977): 39-68 (1978)

▶ Hazardous Substances Data Bank (HSDB)

SURFACE WATER: 2,4-Dimethylphenol has been detected in 1% of 804 samples reported in STORET, EPA's water quality database for 1975-82(1), immediately downstream from waste input into a creek from a former pine-tar manufacturing facility in Gainesville, FL, concn ranging from 10-200 ug/l(2), and in Smith Creek in Sept 1980, near, and shortly after the Mt. St. Helens, WA explosion, but not found in 3 nearby lakes(3). 2,4-Dimethylphenol has also been identified in on-site lagoons at a covered wastefill in Forest Waste, MI, at a concns estimated at 40 and 100 ug/l(4) and in an aqueous sample collected near Quantico, VA, concn <2 ug/l(5).

(1) Staples CA et al; Environ Toxicol Chem 4: 131-42 (1985) (2) McCreary JJ et al; Chemosphere 12: 1619-32 (1983) (3) McKnight DM et al; Org Geochem 4: 85-92 (1982) (4) USEPA; Superfund Record of Decision (EPA Region 5). USEPA/ROD/RO5-86/034. (NTIS PB87-18980) (1986) (5) Hall LWJR et al; Aquat Tox 10: 73-99 (1987)

▶ Hazardous Substances Data Bank (HSDB)

RAIN/SNOW: The concentration of 2,4- and 2,5-dimethylphenol, combined in rainwater for seven events in Portland, OR ranged from 300 to 1300 ng/l, 820 ng/l avg(1).

(1) Leuenberger C et al; Environ Sci Technol 19: 1053-8 (1985)

▶ Hazardous Substances Data Bank (HSDB)

13.2.14 Effluent Concentrations

2,4-Dimethylphenol was detected in raw sludge and treated sludge, concns unknown, in samples taken from 37 water pollution control plants in Ontario, Canada between January and July 1986(1). Waste water from the gasification of Indian Head lignite coal in North Dakota was determined to have an estimated 2,4/2,5-dimethylphenol concn of 368 mg/l(1). A summary of analysis for 2,4-dimethylphenol in effluent reports that it was found 3 times in residential, 8 times in industrial, and 2 times in commercial effluent, with an overall source average discharge concn of 0.7, 0.0, and 74.0 ug/l, respectively(3). 2,4-Dimethylphenol was identified but not quantified in leachate collected from a Swedish municipal landfill in May 1990(4). Groundwater and soil from 91 waste sites at 18 Department of Energy (DOE) facilities were analyzed; 2,4-dimethylphenol was found at one of the facilities in groundwater, concn not quantified(5).

(1) Canviro Consultants; Thirty Seven Municipal Water Pollution Control Plants, Pilot Monitoring Study Volume 1. Interim Report. Ontario Ministry of the Environment Water Resources Branch. ISBN 0-7729-4900-X. pp. 97 (1988) (2) Giabbai MF et al; Int J Environ Anal Chem 20: 113-29 (1985) (3) Levins P et al; Sources of Toxic Pollutants Found in Influents to Sewage Treatment Plants, USEPA-440/4-81-008 (NTIS PB1-219685) (1981) (4) Oman C, Hynning PA; Environ Pollut 80: 265-71 (1993) (5) Riley RG, Zachara JM; Chemical Contaminants of Doe Lands and Selection of Contaminant Mixtures for Subsurface Science Research. Doe/ER-0547T (NTIS DE92014826) Richland,WA: Pac Northwest Lab (1993)

▶ Hazardous Substances Data Bank (HSDB)

2,4-Dimethylphenol was found in six effluents in an EPA survey (4000 samples) of effluents covering 46 industrial categories(1). Industries with positive levels of 2,4-dimethylphenol included iron and steel manufacturing, petroleum refining, organics and plastics, rubber processing, organic chemicals, and publicly owned treatment works(1). 2,4-Dimethylphenol was detected in 3.4% of 1321 effluent samples reported in STORET, EPA's water quality data base (1975-82)(2) and, in two out of five effluents of hazardous waste incinerators(3) and at 10 ug/l in urban runoff in Washington, DC(4). This constituted a 2% frequency of detection in the National Urban Runoff Program, which examined 86 runoff samples from 15 USA cities(4). The final effluent of Los Angeles County Municipal Wastewater Treatment Plant was found to contain 5 and <10 ppb 2,4-dimethylphenol in July 1978 and Nov 1980, respectively(5). Of 18 advanced water treatment effluents analyzed, 2,4-dimethylphenol was found in effluents at Lake Tahoe, CA (2 ng/l) and Blue Plains, WA (1 and 8.9 ng/l)(6).

(1) Bursey JT, Pellizzari ED; Analysis of Industrial Wastewater for Organic Pollut in Consent Degree Survey. USEPA Contract No. 68-03-2867 p. 167 (1982) (2) Staples CA et al; Environ Toxicol Chem 4: 131-42 (1985) (3) James RH et al; Proc APCA Annu Meet Vol.1, pp. 84-18.5 (1984) (4) Cole et al; J Water Pollut Control Fed 56: 898-908 (1984) (5) Young DR et al; 4: 871-84 in Water Chlorination: Environ Impact Health Eff (1983) (6) Lucas SV; GC/MS Analysis of Organics in Drinking Water concentrates and Advanced Waste Treatment Concentrates, Vol.1 p 321 USEPA-600/1-84-020A NTIS PB85-128221 (1984)

▶ Hazardous Substances Data Bank (HSDB)

13.2.15 Sediment/Soil Concentrations

0.3% of 310 samples from STORET (EPA water quality database) stations reported detectable amounts of 2,4-dimethylphenol in sediment in 1975-82(1). 2,4-Dimethylphenol was detected in a soil sample at the site of a former pine-tar manufacturer in Gainesville, FL(2) and in soil on 7 occasions at a closed wood-to-charcoal conversion plant in McKean county, PA, concn ranging from 1100-390,000 ug/kg(3). 2,4-Dimethylphenol was identified at an unauthorized disposal site in Pemberton Township, NJ in two samples of surface soil (avg concn= 220 ug/kg), but was not detected in subsurface soil(4).

(1) Staples CA et al; Environ Toxicol Chem 4: 131-42 (1985) (2) McCreary JJ et al; Chemosphere 12: 1619-32 (1983) (3) USEPA; Superfund Record of Decision (EPA Region 3). USEPA/ROD/RO3-86/024 (1987) (4) USEPA; Superfund Record of Decision (EPA Region 2). USEPA/ROD/RO2-86/031. (NTIS PB87-188470) (1987)

▶ Hazardous Substances Data Bank (HSDB)

13.2.16 Atmospheric Concentrations

URBAN/SUBURBAN: In 1984, a gas phase concn of 2,4-dimethylphenol (combined with 2,5-dimethylphenol) was detected in 7 of seven rain events in Portland, OR, at concns ranging from 15-70 ng/cu m, 33 ng/cu m; the amount associated with adsorption to particulate matter was <5% of the gas phase concn in every case and generally <1% of the gas phase(1). 2,4-Dimethylphenol was detected at 1 ug/cu m in the air outside an oil shale wastewater facility in Logan WA, but not in an undeveloped site in the oil shale region or in Boulder, CO(2). SOURCE DOMINATED: Although found in gasoline and diesel motor exhaust, 2,4-dimethylphenol was not detected in an Allegheny Mountain highway tunnel(3).

(1) Leuenberger C et al; Environ Sci Technol 19: 1053-8 (1985) (2) Hawthorne SB, Sievers RE; Environ Sci Technol 19: 992-7 (1984) (3) Hampton CV et al; Environ Sci Technol 16: 287-98 (1982)

▸ Hazardous Substances Data Bank (HSDB)

13.2.17 Plant Concentrations

A field study of industrial organic uptake by growing crops was conducted during 1990 at the St. David Coal Refuse Pile Reclamation Site, Fulton County, IL; 2,4-dimethylphenol was detected in coal refuse and plant materials, concns unknown(1).

(1) Webber MD et al; J Environ Qual 23: 1019-26 (1994)

▸ Hazardous Substances Data Bank (HSDB)

13.2.18 Fish/Seafood Concentrations

2,4-Dimethylphenol was not detected in 99 samples of fish reported in STORET, EPA's water quality database in 1975-82(1). However, 2,4-dimethylphenol has been qualitatively detected in several varieties of fish collected from Lake Michigan and tributary streams in 1983(2).

(1) Staples CA et al; Environ Toxicol Chem 4: 131-42 (1985) (2) Camanzo J et al; Great Lakes Res 13: 296-309 (1987)

▸ Hazardous Substances Data Bank (HSDB)

13.2.19 Other Environmental Concentrations

IDENTIFIED IN PARTICULATE PHASE OF TOBACCO SMOKE: 2,4- AND 2,5-DIMETHYLPHENOLS, 2000 UG/100 CIGARETTES. /FROM TABLE/

Searle, C. E. (ed.). Chemical Carcinogens. ACS Monograph 173. Washington, DC: American Chemical Society, 1976., p. 356

▸ Hazardous Substances Data Bank (HSDB)

2,4-Dimethylphenol was identified as a component of cigarette smoke, with concns ranging from 0.7 to 2.1 mg/100 cigarettes (analyzed with 2,5-dimethylphenol)(1).

(1) Wynder EL, Hoffmann D; Tobacco and Tobacco Smoke: Studies in Experimental Carcinogenesis. NY,NY: Academic Press (1967)

▸ Hazardous Substances Data Bank (HSDB)

13.2.20 Probable Routes of Human Exposure

Cigarette and marijuana smoking groups and those exposed to cigarette smoke inhale ug quantities of 2,4-dimethylphenol. The NIOSH has estimated that 11,000 people in the USA are occupationally exposed to cresol containing 2,4-dimethylphenol.

Sittig, M. Handbook of Toxic and Hazardous Chemicals and Carcinogens, 1985. 2nd ed. Park Ridge, NJ: Noyes Data Corporation, 1985., p. 368

▸ Hazardous Substances Data Bank (HSDB)

NIOSH (NOES Survey 1981-1983) has statistically estimated that 7,786 workers are potentially exposed to dimethylphenol in the US, isomer not specified(1). Occupational exposure to 2,4-dimethylphenol may occur through inhalation of this compound at workplaces where 2,4-dimethylphenol is produced or used(SRC). The general population may be exposed to 2,4-dimethylphenol via inhalation of ambient air (i.e., tobacco smoke(2) and automobile exhaust(3)), ingestion of food(4), and contact with other products that may contain 2,4-dimethylphenol(5).

(1) NIOSH; National Occupational Exposure Survey (NOES) (1989) (2) Wynder EL, Hoffmann D; Tobacco and Tobacco Smoke: Studies in Experimental Carcinogenesis. NY,NY: Academic Press (1967) (3) Hampton CV et al; Environ Sci Technol 16: 287-98 (1982) (4) Camanzo J et al; Great Lakes Res 13: 296-309 (1987) (5) Kaiser HE; Cancer 20: 614-6 (1966)

▸ Hazardous Substances Data Bank (HSDB)

13.2.21 Body Burden

Urine from 35 varnishing workers in six different workplaces contained an average 2,4-dimethylphenol concn of 3.8 mg/l; phenols are metabolites of benzene and alkyl benzenes in the varnish(1).

PMID:4066054

(1) Angerer J, Wulf H; Int Arch Occup Environ Health 56: 307-21 (1985)

▸ Hazardous Substances Data Bank (HSDB)

14 Associated Disorders and Diseases

▸ Comparative Toxicogenomics Database (CTD)

15 Literature

15.1 NLM Curated PubMed Citations

▸ PubChem

15.2 Springer Nature References

▸ Springer Nature

15.3 Thieme References

- Thieme Chemistry

15.4 Wiley References

- Wiley

15.5 Depositor Provided PubMed Citations

- PubChem

15.6 General References

Zhu et al. Catalytic activation of unstrained C(aryl)-C(aryl) bonds in 2,2 -biphenols. Nature Chemistry, doi: 10.1038/s41557-018-0157-x, published online 5 November 2018

- Nature Chemistry

15.7 Chemical Co-Occurrences in Literature

▸ PubChem

15.8 Chemical-Gene Co-Occurrences in Literature

▸ PubChem

15.9 Chemical-Disease Co-Occurrences in Literature

▸ PubChem

16 Patents

16.1 Depositor-Supplied Patent Identifiers

- PubChem

Link to all deposited patent identifiers

- PubChem

16.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

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

- PATENTSCOPE (WIPO)

17 Biomolecular Interactions and Pathways

17.1 Protein Bound 3D Structures

- RCSB Protein Data Bank (RCSB PDB)

View 1 protein in NCBI Structure

- PubChem

17.1.1 Ligands from Protein Bound 3D Structures

PDBe Ligand Code	N0D
PDBe Structure Code	6ONR
PDBe Conformer	

- Protein Data Bank in Europe (PDBe)

17.2 Drug-Gene Interactions

- Drug Gene Interaction database (DGIdb)

17.3 Chemical-Gene Interactions

17.3.1 CTD Chemical-Gene Interactions

- Comparative Toxicogenomics Database (CTD)

17.4 Pathways

- PubChem

18 Biological Test Results

18.1 BioAssay Results

▸ PubChem

19 Classification

19.1 Ontologies

19.1.1 MeSH Tree

▸ Medical Subject Headings (MeSH)

19.1.2 ChEBI Ontology

▸ ChEBI

19.1.3 ChemIDplus

▸ ChemIDplus

19.1.4 CAMEO Chemicals

▸ CAMEO Chemicals

19.1.5 UN GHS Classification

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

19.1.6 EPA CPDat Classification

▸ EPA Chemical and Products Database (CPDat)

19.1.7 NORMAN Suspect List Exchange Classification

▸ NORMAN Suspect List Exchange

19.1.8 EPA DSSTox Classification

▸ EPA DSSTox

19.1.9 Consumer Product Information Database Classification

▸ Consumer Product Information Database (CPID)

20 Information Sources

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CAMEO Chemical Reactivity Classification
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3. **ChemIDplus**

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2,4-Dimethylphenol
https://chem.nlm.nih.gov/chemidplus/sid/0000105679
ChemIDplus Chemical Information Classification
https://chem.nlm.nih.gov/chemidplus/

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2,4-DIMETHYLPHENOL
https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=3829

5. **EPA Chemicals under the TSCA**

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Phenol, 2,4-dimethyl-
https://www.epa.gov/chemicals-under-tsca

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

2,4-Dimethylphenol
https://comptox.epa.gov/dashboard/DTXSID2021864
CompTox Chemicals Dashboard Chemical Lists
https://comptox.epa.gov/dashboard/chemical_lists/

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

2,4-xylenol
https://echa.europa.eu/substance-information/-/substanceinfo/100.003.020
2,4-xylenol
https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/116343

8. **Hazardous Substances Data Bank (HSDB)**

2,4-DIMETHYLPHENOL

https://pubchem.ncbi.nlm.nih.gov/source/hsdb/4253

9. ILO International Chemical Safety Cards (ICSC)

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> https://www.ilo.org/global/copyright/request-for-permission/lang--en/index.htm

2,4-XYLENOL
https://www.ilo.org/dyn/icsc/showcard.display?p_version=2&p_card_id=0458

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

> LICENSE
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> https://www.cdc.gov/Other/disclaimer.html

2,4-Xylenol
https://www.cdc.gov/niosh-rtecs/ZE557300.html

11. NJDOH RTK Hazardous Substance List

2,4-dimethylphenol
http://nj.gov/health/eoh/rtkweb/documents/fs/0764.pdf

12. ChEBI

2,4-Dimethylphenol
http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:34241

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

13. Comparative Toxicogenomics Database (CTD)

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> http://ctdbase.org/about/legal.jsp

http://ctdbase.org/detail.go?type=chem&acc=C027804

14. Consumer Product Information Database (CPID)

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

2,4-Xylenol
https://www.whatsinproducts.com/chemicals/view/1/6295/000105-67-9

Consumer Products Category Classification
https://www.whatsinproducts.com/

15. Drug Gene Interaction database (DGIdb)

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>
> http://www.dgidb.org/downloads

https://www.dgidb.org/drugs/CHEMBL29878

16. EPA Chemical and Products Database (CPDat)

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

2,4-xylenol
https://comptox.epa.gov/dashboard/DTXSID2021864#exposure

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

17. EU Food Improvement Agents

2,4-Dimethylphenol
https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32012R0872

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

2,4-xylenol
http://hcis.safeworkaustralia.gov.au/HazardousChemical/Details?chemicalID=4717

19. NITE-CMC

2,4-Xylenol - FY2015
https://www.nite.go.jp/chem/english/ghs/15-meti-0025e.html

2,4-Xylenol - FY2006

https://www.nite.go.jp/chem/english/ghs/06-imcg-0513e.html

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> https://www.fda.gov/about-fda/about-website/website-policies#linking

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

21. NORMAN Suspect List Exchange

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2,4-Dimethylphenol

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

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2,4-DIMETHYLPHENOL
http://mona.fiehnlab.ucdavis.edu/spectra/browse?inchikey=KUFFULVDNCHOFZ-UHFFFAOYSA-N

23. NIST Mass Spectrometry Data Center

Phenol, 2,4-dimethyl-
http://www.nist.gov/srd/nist1a.cfm

24. Nature Chemistry

https://pubchem.ncbi.nlm.nih.gov/substance/375798285

25. Protein Data Bank in Europe (PDBe)

http://www.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/N0D

26. RCSB Protein Data Bank (RCSB PDB)

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> https://www.rcsb.org/pages/policies

https://www.rcsb.org/

27. SpectraBase

2,4-XYLENOL
https://spectrabase.com/spectrum/JRb3rHzPVwp

2,4-DIMETHYLPHENOL
https://spectrabase.com/spectrum/6u9UwRwFDgW

2,4-DIMETHYLPHENOL
https://spectrabase.com/spectrum/G8SVr0HYOV

2,4-XYLENOL
https://spectrabase.com/spectrum/LYo8NIIRX35

2,4-Dimethylphenol
https://spectrabase.com/spectrum/DptSLkSbOel

phenol novolac
https://spectrabase.com/spectrum/9SJXuRfeJ0A

phenolnovolac
https://spectrabase.com/spectrum/GX7aYBAxHU8

phenolnovolac
https://spectrabase.com/spectrum/AF30Bo1wKG3

2,4-Dimethylphenol
https://spectrabase.com/spectrum/52Xbq3LB2b2

2,4-DIMETHYLPHENOL
https://spectrabase.com/spectrum/5qTYdxBuuxx

2,4-XYLENOL
https://spectrabase.com/spectrum/Itxq6rQJvjx

2,4-XYLENOL
https://spectrabase.com/spectrum/FMOIaeLYvc0

2,4-DIMETHYLPHENOL
https://spectrabase.com/spectrum/H55FiUMgBPX

2,4-XYLENOLE
https://spectrabase.com/spectrum/56XzEfOCaqJ

PHENOL, 2,4-DIMETHYL-
https://spectrabase.com/spectrum/CUerNyoj15r

2,4-Xylenol
https://spectrabase.com/spectrum/CDnLvM1FDlT

2,4-Xylenol
https://spectrabase.com/spectrum/7oPUx9G8KqV

2,4-Xylenol
https://spectrabase.com/spectrum/Bd4h5BF4Kpe

2,4-Xylenol
https://spectrabase.com/spectrum/5wViyVJockn

2,4-Xylenol
https://spectrabase.com/spectrum/HwykwB18vtb

2,4-Xylenol
https://spectrabase.com/spectrum/CCiAgmvz8B

2,4-Xylenol
https://spectrabase.com/spectrum/IuK0cd7Yd9u

2,4-Xylenol
https://spectrabase.com/spectrum/2ROKgQXQHvR

2,4-Xylenol
https://spectrabase.com/spectrum/FWSX8iCTZj1

2,4-Xylenol
https://spectrabase.com/spectrum/8ihFFSEUeTH

2,4-Xylenol
https://spectrabase.com/spectrum/FxX1TNDTqE6

2,4-Xylenol
https://spectrabase.com/spectrum/AxYFXVhbhZV

2,4-Xylenol
https://spectrabase.com/spectrum/9OswnHnCe3X

2,4-Xylenol
https://spectrabase.com/spectrum/GNxXQ3pd5qZ

2,4-Xylenol
https://spectrabase.com/spectrum/8lYmI79Zn0c

2,4-Xylenol
https://spectrabase.com/spectrum/DoThM7yb5zR

2,4-xylenol
https://spectrabase.com/spectrum/1jC2EqAg24G

2,4-Dimethylphenol
https://spectrabase.com/spectrum/2h6gIeZNhlS

2,4-Dimethylphenol
https://spectrabase.com/spectrum/6FoeYbm0ROG

2,4-Dimethylphenol
https://spectrabase.com/spectrum/4VGEeZtjxfZ

2,4-Dimethylphenol
https://spectrabase.com/spectrum/3KJOSWmXGiy

2,4-Dimethylphenol
https://spectrabase.com/spectrum/LZSSpRxab6L

2,4-Dimethylphenol
https://spectrabase.com/spectrum/1V5sgSxIxVh

Phenol, 2,4-dimethyl-
https://spectrabase.com/spectrum/12LAU2XsGXC

Phenol, 2,4-dimethyl-
https://spectrabase.com/spectrum/A1wSaymNw0F

2,4-DIMETHYLPHENOL
https://spectrabase.com/spectrum/FRk2myJb8M8

2,4-DIMETHYLPHENOL
https://spectrabase.com/spectrum/6NPgVptG9Ze

2,4-Dimethylphenol
https://spectrabase.com/spectrum/6vXV6nbjSYx

Phenol, 2,4-dimethyl-
https://spectrabase.com/spectrum/JCkBd8W9Cgi

Phenol, 2,4-dimethyl-
https://spectrabase.com/spectrum/ASSSHLSyohk

Phenol, 2,4-dimethyl-
https://spectrabase.com/spectrum/GfxYSFNcmqe

Phenol, 2,4-dimethyl-
https://spectrabase.com/spectrum/HJxMAjGK7nc

Phenol, 2,4-dimethyl-
https://spectrabase.com/spectrum/H1oFK3MtWyG

Phenol, 2,4-dimethyl-
https://spectrabase.com/spectrum/5sHsTAx0bse
Phenol, 2,4-dimethyl-
https://spectrabase.com/spectrum/GkxAFDY0mum
Phenol, 2,4-dimethyl-
https://spectrabase.com/spectrum/HYpvlbO6M52
Phenol, 2,4-dimethyl-
https://spectrabase.com/spectrum/FMbIdONYORs

28. Springer Nature
https://pubchem.ncbi.nlm.nih.gov/substance/341151406

29. SpringerMaterials
2,4-xylenol
https://materials.springer.com/substanceprofile/docs/smsid_kwfrqkdracjuidrs

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

Dimethylphenol, 2,4-
https://epa-prgs.ornl.gov/cgi-bin/chemicals/csl_search
Dimethylphenol, 2,4-
https://epa-prgs.ornl.gov/cgi-bin/chemicals/csl_search?tool=rml

32. Wikipedia
2,4-Dimethylphenol
https://de.wikipedia.org/wiki/2,4-Xylenol

33. Wiley
https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=96023

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

35. Medical Subject Headings (MeSH)
2,4-dimethylphenol
https://www.ncbi.nlm.nih.gov/mesh/67027804
MeSH Tree
http://www.nlm.nih.gov/mesh/meshhome.html

36. UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)
GHS Classification Tree
http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

37. PATENTSCOPE (WIPO)
SID 403034541
https://pubchem.ncbi.nlm.nih.gov/substance/403034541