COMPOUND SUMMARY

# 1,2,4-Trichlorobenzene

PubChem CID	13
Structure	Image: Structures
Chemical Safety	Initiant       Initiant         Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub>
Synonyms	1,2,4-trichlorobenzene 120-82-1 Benzene, 1,2,4-trichloro- unsym-Trichlorobenzene Hostetex L-pec More
Molecular Weight	181.4
Dates	Modify Create 2021-07-03 2004-09-16
1,2,4-trichlorobenzene appears CAMEO Chemicals	as colorless liquid or white solid with a sharp chlorobenzene odor. Melting point 16.95°C (62.5°F) . (USCG, 1999)
1,2,4-trichlorobenzene is a trich	lorobenzene with chloro substituents at positions 1, 2 and 4.
ChEBI	
Occupational exposure to 1,2,4- trichlorobenzene in humans. Lo the cortex in rats. Liver effects h EPA Air Toxics	-trichlorobenzene may occur from inhalation during its manufacture and use. No information is available on the acute (short-term), chronic (long-term), reproductive, developmental, and carcinogenic effects of 1,2,4- cal irritation of the lungs and dyspnea have been reported in animals following acute inhalation exposure. Chronic oral exposure has been observed to result in increased adrenal weights and vacuolization of the zona fasciculata in ave also been reported following chronic oral exposure in rats. EPA has classified 1,2,4-trichlorobenzene as a Group D, not classifiable as to human carcinogenicity.

1 Structures	0 Z
1.1 2D Structure	0 2
	53
Chemical Structure Depiction	
	+ _
PubChem	

1.2 3D Conformer	0 Z

2 Names and Identifiers	0 2
2.1 Computed Descriptors	0 2
2.1.1 IUPAC Name	0 2
1,2,4-trichlorobenzene Computed by LexiChem 2.6.6 (PubChem release 2019.06.18) ▶ PubChem	
2.1.2 InChI	0 2
InChI=15/C6H3Cl3/c7-4-1-2-5(8)6(9)3-4/h1-3H Computed by InChI 1.0.5 (PubChem release 2019.06.18) PubChem	
2.1.3 InChI Key	0 2
PBKONEOXTCPAFI-UHFFFAOYSA-N Computed by InChI 1.0.5 (PubChem release 2019.06.18) PubChem	
2.1.4 Canonical SMILES	0 2
C1=CC(=C(C=C1CI)CI)CI Computed by OEChem 2.1.5 (PubChem release 2019.06.18) PubChem	
2.2 Molecular Formula	0 🛛
C6H3Cl3 CAMEO Chemicals; ILO International Chemical Safety Cards (ICSC); PubChem	
2.3 Other Identifiers	0 2
2.3.1 CAS	0 2
120-82-1 CAMEO Chemicals; CAS Common Chemistry; ChemIDplus; DTP/NCI; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA); Hazardous Substances Da	ata Bank (HSDB); ILO International Chemical Safety Cards (ICSC); Occupational Safety and Health Administration (OSHA
63697-18-7	
2.3.2 European Community (EC) Number	0 2
204-428-0 European Chemicals Agency (ECHA)	
2.3.3 ICSC Number	

	? Z
1049	
ILO International Chemical Safety Cards (ICSC)	
	<u> </u>
2.3.4 NSC Number	00
406697	
DTP/NCI	
2.3.5 RTECS Number	? Z
DC2100000	
The National Institute for Occupational Safety and Health (NIOSH)	
	<u>م</u> ۲۵
2.3.6 UN Number	ڭ ( <sup>2</sup> )
2321	
CAMEO Chemicals; ILO International Chemical Safety Cards (ICSC); NJDOH RTK Hazardous Substance List; The National Institute for Occupational Safety and Health (NIOSH)	
2.3.7 UNII	? Z
05IQ959M1N	
FDA/SPL Indexing Data	
	0 7
	<u> </u>
2.3.9 Wikipedia	0 Z
1,2,4-trichlorobenzene	
▶ Wikipedia	
2.4 Synonyms	0 2
2.4.1 MeSH Entry Terms	(?) Z
1.2.4-trichlorobenzene	02
Medical Subject Headings (MeSH)	

2.4.2 Depositor-Supplied Synonyms					0 Z		
1,2,4-trichlorobenzene	1,2,4-trichloro-benzene	Trojchlorobenzen [Polish]	1,4-Trichlorobenzol	2,4-dichlorophenyl chloride	Tox21_300563	NCGC00090833-02	1,2,4-Trichlorobenzene, for HPLC, >=99%
120-82-1	Trichlorobenzene A	1,2,4-Trichlorobenzene, 99%, pure	1,4-Trichlorobenzene	SCHEMBL22730	ANW-17536	NCGC00090833-03	1,2,4-Trichlorobenzene, for synthesis, 99%
Benzene, 1,2,4-trichloro-	NSC 406697	CAS-120-82-1	63697-18-7	ghl.PD_Mitscher_leg0.137	NSC406697	NCGC00090833-04	C06594
unsym-Trichlorobenzene	UNII-05IQ959M1N	CCRIS 5945	1,2,4-triclorobenzene	MLS001050173	SBB060225	NCGC00254336-01	1,2,4-Trichlorobenzene 100 microg/mL in Hexane
Hostetex L-pec	1,2,4-TCB	HSDB 1105	Benzene,2,4-trichloro-	BIDD:ER0328	STL481897	NCGC00258863-01	1,2,4-Trichlorobenzene, ReagentPlus(R), >=99%

https://pubchem.ncbi.nlm.nih.gov/compound/13#section=Safety-and-Hazards

### 1,2,4-Trichlorobenzene | C6H3Cl3 - PubChem

Trojchlorobenzen	MFCD00000547	EINECS 204-428-0	ACMC-1B7LJ	CHEMBL296348	AKOS000120900	S697	1,2,4-Trichlorobenzene, Spectrophotometric Gra         Benzene,1,2,4-trichloro-,radical ion(1-)(9ci)         J-503791         Q1876830         1,2,4-Trichlorobenzene 10 microg/mL in Cyclohe:         1,2,4-Trichlorobenzene 5000 microg/mL in Meth
1,2,4-Trichlorbenzol	CHEBI:28222	BRN 0956819	WLN: GR BG DG	DTXSID0021965	MCULE-2714956388	SMR001216523	
1,2,4-Trichlorobenzol	05IQ959M1N	1, 2, 4-Trichlorobenzene	bmse000841	124-TCB	NE10031	1,2,4-Trichlorobenzene, anhydrous, >=99	
1,3,4-Trichlorobenzene	DSSTox_CID_1965	Trichlorobenzol	UN 2321 (Related)	ZINC388208	NSC-406697	FT-0606243	
1,2,5-Trichlorobenzene	DSSTox_RID_76431	Al3-07775	Benzene, 1,2,4-trichloro-, radical ion(1-)	AMY40773	1,2,4-TRICHLOROBENZENE (D3)	FT-0606251	
as-trichlorobenzene	DSSTox_GSID_21965	Hipochem GM	EC 204-428-0	Tox21_201311	NCGC00090833-01	ST50406605	
4		·					•

PubChem

# **3** Chemical and Physical Properties

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## **3.1 Computed Properties**

Property Name	Property Value	Reference
Molecular Weight	181.4	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3	4	Computed by XLogP3 3.0 (PubChem release 2019.06.18)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	0	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	179.930033	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	179.930033	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	0 Ų	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	94.3	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

#### I.L.D. 3

3.2 Experimental Properties	? 🛽
3.2.1 Physical Description	0 Z

1,2,4-trichlorobenzene appears as colorless liquid or white solid with a sharp chlorobenzene odor. Melting point 16.95°C (62.5°F). (USCG, 1999)

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

#### CAMEO Chemicals

Liquid

#### EPA Chemicals under the TSCA

COLOURLESS LIQUID OR WHITE CRYSTALS WITH CHARACTERISTIC ODOUR.

ILO International Chemical Safety Cards (ICSC)

Colorless liquid or crystalline solid (below 63°F) with an aromatic odor.

• Occupational Safety and Health Administration (OSHA); The National Institute for Occupational Safety and Health (NIOSH)

#### 3.2.2 Color/Form

Colorless liquid

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1265

Hazardous Substances Data Bank (HSDB)

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#### Orthorhombic crystals

Lide, D.R. CRC Handbook of Chemistry and Physics 88TH Edition 2007-2008. CRC Press, Taylor & Francis, Boca Raton, FL 2007, p. 3-492

#### Hazardous Substances Data Bank (HSDB)

#### Colorless liquid or crystalline solid (below 63 degrees F).

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases CD-ROM. Department of Health & Human Services, Centers for Disease Prevention & Control. National Institute for Occupational Safety & Health. DHHS (NIOSH) Publication No. 2005-151 (2005)

#### Hazardous Substances Data Bank (HSDB)

3.2.3 Odor	0 Z
Aromatic odor NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases CD-ROM. Department of Health & Human Services, Centers for Disease Prevention & Control. National Institute for Occupational Safety & Health. DHHS (NIOSH) Publication No. 2005-151 (2005) Hazardous Substances Data Bank (HSDB)	
3.2.4 Boiling Point	0 2
415 °F at 760 mm Hg (NTP, 1992)	

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

#### CAMEO Chemicals

#### 213.5 °C

#### EPA DSSTox; Hazardous Substances Data Bank (HSDB)

213 °C

#### ILO International Chemical Safety Cards (ICSC)

#### 416°F

Occupational Safety and Health Administration (OSHA); The National Institute for Occupational Safety and Health (NIOSH)

|--|

#### 63 °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

#### 17.0 °C

#### EPA DSSTox

#### 16.92 °C

Lide, D.R. CRC Handbook of Chemistry and Physics 88TH Edition 2007-2008. CRC Press, Taylor & Francis, Boca Raton, FL 2007, p. 3-492

#### Hazardous Substances Data Bank (HSDB)

#### 17 °C

ILO International Chemical Safety Cards (ICSC)

#### 63°F

Cccupational Safety and Health Administration (OSHA); The National Institute for Occupational Safety and Health (NIOSH)

#### 3.2.6 Flash Point

#### 230 °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

#### 105 °C (222 °F)

Fire Protection Guide to Hazardous Materials. 13 ed. Quincy, MA: National Fire Protection Association, 2002., p. 325-109

#### Hazardous Substances Data Bank (HSDB)

105 °C c.c.

#### ILO International Chemical Safety Cards (ICSC)

#### 222°F

• Occupational Safety and Health Administration (OSHA); The National Institute for Occupational Safety and Health (NIOSH)

#### 3.2.7 Solubility

#### less than 1 mg/mL at 70° 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

#### 2.70e-04 M

SOUTHWORTH,GR & KELLER,JL (1986)

#### EPA DSSTox

#### Sparingly soluble in alcohol. Miscible with ether, benzene, petroleum ether, carbon disulfide

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1655

#### Hazardous Substances Data Bank (HSDB)

#### In water, 49.0 mg/L at 25 °C

Southwick GR, Keller JL; Water Air Soil Pollut 28: 239-48 (1986)

#### Hazardous Substances Data Bank (HSDB)

#### Solubility in water, mg/l: 34.6

#### ILO International Chemical Safety Cards (ICSC)

#### 0.003%

The National Institute for Occupational Safety and Health (NIOSH)

#### 3.2.8 Density

#### 1.454 at 68 °F (USCG, 1999)

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

#### CAMEO Chemicals

#### 1.459 g cu cm at 20 °C/4 °C

Lide, D.R. CRC Handbook of Chemistry and Physics 88TH Edition 2007-2008. CRC Press, Taylor & Francis, Boca Raton, FL 2007, p. 3-492

Hazardous Substances Data Bank (HSDB)

#### 1,2,4-Trichlorobenzene | C6H3Cl3 - PubChem

#### Liquid density: 1.44829 kg/L

Krishnamurti R; Kirk-Othmer Encyclopedia of Chemical Technology. (2001). NY, NY: John Wiley & Sons; Chlorinated Benzenes. Online Posting Date: Jul 13, 2001.

#### Hazardous Substances Data Bank (HSDB)

#### Critical density: 0.447 kg/L

Krishnamurti R; Kirk-Othmer Encyclopedia of Chemical Technology. (2001). NY, NY: John Wiley & Sons; Chlorinated Benzenes. Online Posting Date: Jul 13, 2001.

Hazardous Substances Data Bank (HSDB)

#### Relative density (water = 1): 1.5

ILO International Chemical Safety Cards (ICSC)

#### 1.45

> Occupational Safety and Health Administration (OSHA); The National Institute for Occupational Safety and Health (NIOSH)

#### 3.2.9 Vapor Density

#### 6.26 (NTP, 1992) (Relative to Air)

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

#### CAMEO Chemicals

#### 6.26 (Air= 1)

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 10th ed. Volumes 1-3 New York, NY: John Wiley & Sons Inc., 1999., p. V3: 3523

#### Hazardous Substances Data Bank (HSDB)

#### Relative vapor density (air = 1): 6.26

#### ILO International Chemical Safety Cards (ICSC)

#### 6.26

Occupational Safety and Health Administration (OSHA)

#### 3.2.10 Vapor Pressure

#### 1 mm Hg at 101.1 °F ; 5 mm Hg at 153.1° 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

#### 0.46 mmHg

#### EPA DSSTox

#### 0.46 mm Hg at 25 °C

Shiu WY, Mackay D; J Chem Eng Data 42: 27-30 (1997)

#### Hazardous Substances Data Bank (HSDB)

Vapor pressure, Pa at 25 °C: 40

ILO International Chemical Safety Cards (ICSC)

#### 1 mmHg

Occupational Safety and Health Administration (OSHA); The National Institute for Occupational Safety and Health (NIOSH)

02

# 02

# 3.2.11 LogP

# 4.02 (LogP)

HANSCH,C ET AL. (1995)

## EPA DSSTox

#### log Kow = 4.02

Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995., p. 16

#### Hazardous Substances Data Bank (HSDB)

#### 3.98

ILO International Chemical Safety Cards (ICSC)

3.2.12 LogKoa	? 🛛
4.95 (Octanol-Air partition coefficient)	
► EPA DSSTox	
3.2.13 Henrys Law Constant	? Z
0.00 atm-m3/mole	
► EPA DSSTox	
Henry's Law constant = 1.42X10-3 atm-cu m/mol at 25 °C Warner HP et al; Determination of Henry's Law constants of selected priority pollutants. EPA/600/D-87/229, NTIS PB87-212684 (1987)	
Hazardous Substances Data Bank (HSDB)	
3.2.14 Atmospheric OH Rate Constant	0 Z
5.50e-13 cm3/molecule*sec KWOK,ESC & ATKINSON,R (1994)	
► EPA DSSTox	
3.2.15 Stability/Shelf Life	0 Z
Stable at room temperature American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values and Biological Exposure Indices. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991., p. 1605 Hazardous Substances Data Bank (HSDB)	

#### Volatile with steam

Budavari, S. (ed.). The Merck Index - Encyclopedia of Chemicals, Drugs and Biologicals. Rahway, NJ: Merck and Co., Inc., 1989., p. 1516

#### Hazardous Substances Data Bank (HSDB)

3.2.16 Autoignition Temperature	? Z
1060 °F (USCG, 1999)	

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

#### CAMEO Chemicals

571 °C (1060 °F)

Fire Protection Guide to Hazardous Materials. 13 ed. Quincy, MA: National Fire Protection Association, 2002., p. 325-109

#### Hazardous Substances Data Bank (HSDB)

#### 571 °C

#### ILO International Chemical Safety Cards (ICSC)

3.2.17 Decomposition	
When heated to decomp, it emits toxic fumes of /hydrogen chloride/. Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 3229 Harardous Substances Data Bank (HSDB)	
3.2.18 Heat of Vaporization	02
280 J/g Krishnamurti R; Kirk-Othmer Encyclopedia of Chemical Technology. (2001). NY, NY: John Wiley & Sons; Chlorinated Benzenes. Online Posting Date: Jul 13, 2001. Hazardous Substances Data Bank (HSDB)	
3.2.19 Odor Threshold	? Z
Industrial data report an odor threshold of approx 3 ppm American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values and Biological Exposure Indices. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991., p. 1605 Hazardous Substances Data Bank (HSDB)	
Low odor threshold= 24.0 mg/cu m; High odor threshold= 24.0 mg/cu m; Irritating concn= 40.0 mg/cu m Ruth JH; Am Ind Hyg Assoc J 47: A-142-51 (1986)	
Hazardous Substances Data Bank (HSDB)	
3.2.20 Refractive Index	0 Z
Index of refraction: 1.5717 at 20 °C/D Lide, D.R. CRC Handbook of Chemistry and Physics 88TH Edition 2007-2008. CRC Press, Taylor & Francis, Boca Raton, FL 2007, p. 3-492	

3.2.21 Kovats Retentio	n Index	0 2
Standard non-polar	1141.6, 1158.5, 1150, 1157, 1162, 1168, 1152, 1160, 1193, 1177, 1193, 1177, 1183, 1193, 1177, 1186, 1161, 1166, 1177, 1187.6, 1161.4, 1148.7, 1175.5, 1174, 1158, 1145, 1142, 1144, 1145, 1149, 1147.1, 1155.4, 1150, 1150, 1154	
Semi-standard non-polar	1192.67, 1193.06, 1196.72, 1196.78, 1172, 1160.14, 1166.23, 1171.69, 1193.56, 1193.67, 1189.6, 1199.7, 1211.1, 1164.56, 1176.18, 1189.56, 1198, 1203.2, 1170, 1198, 199, 198.2	
Standard polar	1643.59, 1658.54, 1659.76, 1671.43, 1665.5, 1688.6, 1630, 1630, 1653, 1698, 1653.9	

#### NIST Mass Spectrometry Data Center

# 3.2.22 Other Experimental Properties

#### Lide, D.R. CRC Handbook of Chemistry and Physics 88TH Edition 2007-2008. CRC Press, Taylor & Francis, Boca Raton, FL 2007, p. 6-128

#### Hazardous Substances Data Bank (HSDB)

#### Standard heat of formation of liquid: -263.1 J/g

Krishnamurti R; Kirk-Othmer Encyclopedia of Chemical Technology. (2001). NY, NY: John Wiley & Sons; Chlorinated Benzenes. Online Posting Date: Jul 13, 2001.

#### Hazardous Substances Data Bank (HSDB)

#### Hydroxyl radical reaction rate constant = 5.50X10-13 cu cm/molec-sec at 25 $^{\circ}\mathrm{C}$

Kwok ESC, Atkinson R; Estimation of hydroxyl radical reaction rate constants for gas-phase organic compounds using a structure-reactivity relationship: an update. Riverside, CA: Univ CA, Statewide Air Pollut Res Ctr. CMA Contract No. ARC-8.0-OR (1994)

#### Hazardous Substances Data Bank (HSDB)

# 3.3 SpringerMaterials Properties

13C nuclear magnetic resonance spectrum	Nuclear quadrupole resonance spectroscopy	Vapor pressure
Boiling point	Optical coefficient	Vapor-liquid equilibrium
Chemical shift	Phase diagram	Viscosity
Density	Phase equilibrium	
Diamagnetic susceptibility	Phase transition	
Dielectric constant	Quadrupole coupling	
Excess enthalpy	Refractive index	
Fusion temperature	Sound absorption	
Heat of solution	Sound propagation	
Heat of sublimation	Sound velocity	
Magnetic susceptibility	Spin-spin coupling constant	
Melting temperature	Thermal expansion coefficient	
Mixing enthalpy	Transition enthalpy	

SpringerMaterials

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# **4** Spectral Information

4 Spectral Info	ormation	0 Z
4.1 1D NMR Spec	tra	0 Z
1D NMR Spectra	1H NMR: 221 (Sadtler Research Laboratories Spectral Collection)	

#### Hazardous Substances Data Bank (HSDB)

1D NMR Spectra	NMRShiftDB Link
NMRShiftDB	

# 4.1.1 1H NMR Spectra

Instrument Name	Varian A-60
Source of Sample	HOOKER CHEMICAL CORPORATION, NIAGARA FALLS, NEW YORK
Copyright	Copyright © 2009-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

#### SpectraBase

### 4.1.2 13C NMR Spectra

Showing 2 of 13 View More

Source of Sample	MCB Manufacturing Chemists, Norwood, Ohio
Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

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Copyright	t

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

#### Thumbnail

#### SpectraBase

# 4.2 Mass Spectrometry

# Showing 2 of 15 View More

Showing 2 of 15 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		

Instrument Name	311A
Source of Spectrum	Chemical Concepts, A Wiley Division, Weinheim, Germany
Copyright	Copyright © 2002-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

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### 4.2.1 GC-MS

# ⊘ℤ

Showing 2 of 7 View More		
MoNA ID	JP000951	
MS Category	Experimental	
MS Type	GC-MS	
MS Level	MS1	
Instrument	JEOL JMS-01-SG	
Instrument Type	El-B	
Ionization Mode	positive	
Top 5 Peaks	180         182       96.3         184       30.2         145       29.0         109       22.1	
SPLASH	splash10-001i-290000000-c9cb3f8f606230da9665	
Thumbnail		
Submitter	University of Tokyo Team, Faculty of Engineering, University of Tokyo	
MassBank of North America (MoNA)		
MoNA ID	JP003622	
MS Category	Experimental	
MS Type	GC-MS	

MS Level	MS1
Instrument	Unknown
Instrument Type	EI-B
Ionization Mode	positive
	180 100
	182 97.2
Top 5 Peaks	184 31.4
	145 22.9
	147 15.5
SPLASH	splash10-001i-190000000-a89e54cbf388d5ac3650
Thumbnail	
Submitter	University of Tokyo Team, Faculty of Engineering, University of Tokyo

MassBank of North America (MoNA)

4.2.2	Other	MS
T. C. C	ounci	1413

		<b>—</b>
Other MS	MASS: 27871 (NIST/EPA/MSDC) Mass Spectral database, 1990 version); 1221 (Atlas of Mass Spectral Data, John Wiley & Sons, New York)	
Hazardous Substance	es Data Bank (HSDB)	
4.3 UV Spectra		? Z

# UV: 1277 (Sadtler Research Laboratories Spectral Collection)

Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V2: 1251

Hazardous Substances Data Bank (HSDB)

4.4 IR Spectra		0 2	
IR Spectra	IR: 4783 (Coblentz Society Spectral Collection)		
Hazardous Substances Data Bank (HSDB)			

4.4.1 FTIR Spectra		0 2
Showing 2 of 6 View More	re 🚺	
Technique	BETWEEN SALTS	
Source of Sample	Hooker Chemical Corporation	
Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.	

https://pubchem.ncbi.nlm.nih.gov/compound/13#section=Safety-and-Hazards

Instrument Name	PERKIN-ELMER 1710
Technique	NEAT
Source of Sample	Environmental Protection Agency
Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

# 4.4.2 ATR-IR Spectra

Showing 2 of 3 View More

Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DuraSamplIR II)
Source of Spectrum	Forensic Spectral Research
Source of Sample	Fluka, Sigma-Aldrich Company Llc.
Catalog Number	36627
Lot Number	SZB9029XV
Copyright	Copyright © 2014-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

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Source of Sample	Sigma-Aldrich
Catalog Number	132047
Copyright	Copyright © 2018-2020 Sigma-Aldrich Co. LLC Database Compilation Copyright © 2018-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	
SpectraBase	

#### 4.4.3 Near IR Spectra

4.4.3 Near IR Spectra		0 2
Technique	NIR Path Length= 0.5/20 Spectrometer= BRUKER IFS 88	
Source of Spectrum	Prof. Buback, University of Goettingen, Germany	
Copyright	Copyright © 1989, 1990-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.	
Thumbnail		

Technique	NIR Path Length= 0.5/20 Spectrometer= BRUKER IFS 88
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	

#### 4.4.4 Vapor Phase IR Spectra

Raman Spectra

Technique	Vapor Phase	
Source of Sample	Fluka Chemie AG, Buchs, Switzerland	
Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.	
Thumbnail		
SpectraBase		
4.5 Raman Spectra	ra	? Z
Showing 2 of 4 View More	7	

Raman: 90 (Dollish et al., Characteristic Raman Frequencis of Organic Compounds, John Wiley & Sons, New York)

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#### Hazardous Substances Data Bank (HSDB)

Instrument Name	Thermo Nicolet FT-Raman 960
Technique	FT-Raman
Source of Sample	Aldrich Chemical Company, Inc.,
Copyright	Copyright © 2003-2020 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	
SpectraBase	

# 4.6 Other Spectra

Intense mass spectral peaks: 180 m/z (100%), 182 m/z (96%), 184 m/z (30%), 145 m/z (30%) Hites, R.A. Handbook of Mass Spectra of Environmental Contaminants. Boca Raton, FL: CRC Press Inc., 1985., p. 73

Hazardous Substances Data Bank (HSDB)

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5 Related Records	0 Z
5.1 Related Compounds with Annotation	0 Z

# 5.2 Related Compounds

Same Connectivity4 RecordsSame Parent, Connectivity19 RecordsSame Parent, Exact16 RecordsMixtures, Components, and<br/>Neutralized Forms1 RecordsSinilar Connection98 RecordsSinilar Conformers4,501 Records

PubChem

5.3 Substan	nces	0 Z
5.3.1 Related S	Substances	0 2
All	225 Records	
Same	168 Records	
Mixture	57 Records	
PubChem		

.3.2 Substances by Category	0 E

⊘ℤ

	5.4 Entrez Crosslin	inks	0 Z
PubMed 170 Records	PubMed	170 Records	
Taxonomy 4 Records	Taxonomy	4 Records	
Gene 10 Records	Gene	10 Records	

PubChem

# 7 Pharmacology and Biochemistry

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[7]

#### 7.1 Absorption, Distribution and Excretion

More than 60% of oral doses of 14C-1,2,4-trichlorobenzene (ca. 21 mg/kg) administered to rats were excreted in bile as S-trichlorophenyl-mercapturic acid pathway metabolites. The biliary metabolites were ultimately excreted in urine mainly as the isomeric mercapturic acids. An acetylated glutathione conjugate was isolated as a major metabolite in bile (8% dose). The acetyl group was shown by mass spectrometry to be on the glutamyl moiety. A glutamylcysteine conjugate of trichlorobenzene was also isolated from bile as a major metabolite (8% dose). Trichlorothiophenols were deduced not to be intermediates or end-products of enzymic metabolism of trichlorobenzene in rats because 14C-2,4,5-trichlorothiophenol dosed ip to rats was excreted as the S-glucuronide (17% dose) and as S-(methylsulphonyl-dichlorophenyl)-mercapturic acid (36% dose).

#### PMID:1632109

Bakke JE et al; Xenobiotica 22 (2): 199-210 (1992).

Hazardous Substances Data Bank (HSDB)

1,2,4-Trichlorobenzene was fed to rats for 7 days at a dose of 1 mmol/kg per day. (14)C-Trichlorobenzene was admin and disposition of the radioactivity was determined. Tissue analysis showed highest levels in fat. Some was excreted in the urine, and fecal excretion was only 5-10% of the dose.

#### PMID:7420477

Smith EN, Carlson GP; J Toxicol Environ Health 6 (4): 737-49 (1980)

#### Hazardous Substances Data Bank (HSDB)

(14)C-labeled 1,2,4-trichlorobenzene was admin orally (10 mg/kg) and iv (10 mg/kg) to rats and rhesus monkeys. By 24 hr, the monkey had excreted 22% of the iv dose and roughly 40% of the oral dose in the urine. Less than 1% of the radioactivity was found in the feces. For the rat, 84% of the oral dose and 78% of the iv dose were collected in the urine by 24 hr; 11% and 7%, respectively, were the amounts collected in the feces.

#### PMID:6124398

Lingg RD et al; Drug Metab Dispos 10 (2): 134-41 (1982)

#### Hazardous Substances Data Bank (HSDB)

Fingerling rainbow trout (Salmo gairdnerii) were exposed to (14)C-labeled 1,2,4-trichlorobenzene for 8 hr in a static exposure (0.018 mg/L) or for 35 days in a continuous-flow exposure (0.20 mg/L) followed by a subsequent elimination period. For 2 days after 8 hr exposure, half-time of elimination of (14)C from muscle & liver was 0.4 days, while after 35 day exposure an early rapid elimination of (14)C from these tissues (half-time= 0.4 days) was followed by slower elimination (half-time= 50 days) during days 4-36. Values for bile were much greater, reaching 240 after 8 hr exposure & 1400 during the 35 day exposure. When larger trout & carp were exposed to (0.2-0.4 mg/L), the bioconcentration factor for bile (14)C to water (14)C was less than 100. Pretreatment of trout with beta-naphthoflavone, an inducer of hepatic mixed-function oxidase, incr this bioconcentration factor for bile to several hundred. Solvent partitioning and thin layer chromatography indicated that about 60% of (14)C in bile from control trout or carp was present as highly polar biotransformation products, while for induced trout the value was more than 90%.

#### PMID:7420471

Melancon MJ, Lech JJ; J Toxicol Environ Health 6 (3): 645-58 (1980)

Hazardous Substances Data Bank (HSDB)

For more Absorption, Distribution and Excretion (Complete) data for 1,2,4-TRICHLOROBENZENE (10 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

#### 7.2 Metabolism/Metabolites

0 Z

More than 60% of oral doses of 14C-1,2,4-trichlorobenzene (ca. 21 mg/kg) administered to rats were excreted in bile as S-trichlorophenyl-mercapturic acid pathway metabolites. The biliary metabolites were ultimately excreted in urine mainly as the isomeric mercapturic acids. An acetylated glutathione conjugate was isolated as a major metabolite in bile (8% dose). The acetyl group was shown by mass spectrometry to be on the glutamyl moiety. A glutamylcysteine conjugate of trichlorobenzene was also isolated from bile as a major metabolite (8% dose). Trichlorothiophenols were deduced not to be intermediates or end-products of enzymic metabolism of trichlorobenzene in rats because 14C-2,4,5-trichlorothiophenol dosed ip to rats was excreted as the S-glucuronide (17% dose) and as S-(methylsulphonyl-dichlorophenyl)-mercapturic acid (36% dose).

PMID:1632109

Bakke JE et al; Xenobiotica 22 (2): 199-210 (1992).

#### Hazardous Substances Data Bank (HSDB)

Microsomal metabolism of 1,2,4-(14C)trichlorobenzene (1,2,4-TrCB) ... was studied with special emphasis on the conversion-dependent covalent binding to protein and DNA. 1,2,4-TrCB was metabolized to 2,3,6- and 2,4,5-trichlorophenol, and trichlorohydroquinones. About 10% of all metabolites became covalently bound to protein in a rather nonselective way. For 1,2,4-TrCB ... a strong correlation between secondary metabolism to hydroquinones and covalent binding was established. Protein binding was completely inhibited by the addition of ascorbic acid, indicating quinone metabolites as the sole reactive species formed. 1,2,4-TrCB ... alkylated DNA, although to a much lesser extent than protein (0.5% ... of all metabolites). Nonquinone intermediates, presumably epoxides, were responsible for a minor portion of the observed DNA binding, since complete inhibition by ascorbic acid was not reached. The differential role of cytochrome P450 both in primary and in secondary metabolism was demonstrated by the use of microsomes from rats pretreated with different inducers. Dexamethasone (DEX) microsomes (cytochrome P450IIIA1) showed the highest activity toward these chlorinated benzenes (14 mol/mg/5 min for 1,2,4-TrCB ... aboth with regard to the formation of protein-bound metabolites. In addition, DEX microsomes preferentially formed 2,3,6-trichlorophenol as the major isomer. The present study clearly demonstrates the high alkylating potency of secondary quinone metabolites derived from chlorinated benzenes and poses a need for reevaluation of the role of epoxides in the observed toxicity of these compounds.

#### PMID:2017752

den Besten C et al; Toxicol Appl Pharmacol; 108 (2): 223-33 (1981).

#### 1,2,4-Trichlorobenzene | C6H3Cl3 - PubChem

#### Hazardous Substances Data Bank (HSDB)

2,3,5- and 2,4,5-trichlorophenyl methyl sulfides, 2,3,5- and 2,4,5-trichlorophenyl methyl sulfoxides, and 2,3,5- and 2,4,5-trichlorophenyl methyl sulfoxed, and adipose tissue were observed. On the other hand, 2,3,5-TCPSO2Me appeared in blood, liver, kidneys, and adipose tissue and remained detectable in the blood and the three tissues until 120 hr. The increases in the activities of aminopyrine N-demethylase and aniline hydroxylase and the contents of cytochromes P450 and b5 in hepatic microsomes produced by 1,2,4-TCB occurred after increases in the hepatic concentration of 2,3,5-TCPSO2Me as 2,3,5-TCPSO2Me increased the above four parameters in rat liver microsomes. The inducing intensity of 2,3,5-TCPSO2Me was their the antibiotic-pretreated rats dosed with 1,2,4-TCB as injected ip into bile duct-cannulated rats, little 2,3,5-TCPSO2Me was detected in blood, liver, kidneys, and adipose tissue. In the antibiotic-pretreated rats dosed with 1,2,4-TCB, 2,3,5-TCPSO2Me was detected in blood, liver, kidneys, and adipose tissue. In the antibiotic-pretreated rats dosed with 1,2,4-TCB, 2,3,5-TCPSO2Me was detected in blood, liver, kidneys, and adipose tissue. In the antibiotic-pretreated rats dosed with 1,2,4-TCB, 2,3,5-TCPSO2Me was detected in blood, liver, kidneys, and adipose tissue. In the antibiotic-pretreated rats dosed with 1,2,4-TCB, 2,3,5-TCPSO2Me was detected in blood, liver, kidneys, and adipose tissue. In the antibiotic-pretreated rats dosed with 1,2,4-TCB, 2,3,5-TCPSO2Me was detected in blood, liver, kidneys, and adipose tissue. In the antibiotic-pretreated rats dosed with 1,2,4-TCB, 2,3,5-TCPSO2Me was detected in blood, liver, kidneys, an

#### PMID:8212004

Kato Y et al; Toxicol Appl Pharmacol 122 (2): 214-21 (1993).

#### Hazardous Substances Data Bank (HSDB)

1,2,4-Trichlorobenzene was reductively converted into monochlorobenzenes, or p-dichlorobenzenes on incubation with intestinal contents of rats. The amounts of monochlorobenzene produced from o-dichlorobenzenes, m-dichlorobenzenes, or p-dichlorobenzenes, as substrates were compared, /and/ ... o-dichlorobenzenes /produced the least amount of monochlorobenzene/. This was consistent with the finding that o-dichlorobenzenes tended to accumulate more than the other isomers. *Tsuchiya T, Yamaha T; Aqric Biol Chem 47 (5): 1163-5 (1983)* 

#### Hazardous Substances Data Bank (HSDB)

For more Metabolism/Metabolites (Complete) data for 1,2,4-TRICHLOROBENZENE (10 total), please visit the HSDB record page.

#### Hazardous Substances Data Bank (HSDB)

1,2,4-trichlorobenzene has known human metabolites that include 2,3,5-trichlorophenol, 2,3,6-trichlorophenol, and 2,4,5-trichlorophenol.

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

#### NORMAN Suspect List Exchange

7.3 Biological Half-Life			

#### Fish Biotrans. Half-Life (Km)

15.85 Days

#### EPA DSSTox

Fingerling rainbow trout (Salmo gairdnerii) were exposed to (14)C-labeled 1,2,4-trichlorobenzene for 8 hr in a static exposure (0.018 mg/L) or for 35 days in a continuous-flow exposure (0.20 mg/L) followed by a subsequent elimination period. For 2 days after 8 hr exposure, half-time of elimination of (14)C from muscle & liver was 0.4 days, while after 35 day exposure an early rapid elimination of (14)C from these tissues (half-time= 0.4 days) was followed by slower elimination (half-time= 50 days) during days 4-36.

#### PMID:7420471

Melancon MJ, Lech JJ; J Toxicol Environ Health 6 (3): 645-58 (1980)

#### Hazardous Substances Data Bank (HSDB)

In a tissue distribution study groups of rats were given 1.36 mmol 1,2,4-TCB/kg intraperitoneally and animals were killed at intervals up to 120 hours after dosing. The estimated half-lives of 1,2,4-TCB in blood, liver and kidney were 5.8, 5.2, and 6.2 hours, respectively. The 1,2,4-TCB levels were much higher in adipose tissue than in blood and other tissues.

European Chemicals Bureau; European Union Risk Assessment Report, 1,2,4-Trichlorobenzene (120-82-1) (2003). Available from query page, as of July 7, 2009: https://esis.jrc.ec.europa.eu/

#### Hazardous Substances Data Bank (HSDB)

#### 7.4 Biochemical Reactions

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Rhea - Annotated Reactions Database

PubChem

7.5 Transformations

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NORMAN Suspect List Exchange

8 Use and Manufacturing	0 2
8.1 Use Classification	0 2
Hazardous Air Pollutants (HAPs)	

#### EPA Air Toxics

#### 8.2 Uses

1,2,4-Trichlorobenzene is used as a dye carrier, a herbicide intermediate, a heat-transfer medium, a dielectric fluid in transformers, a degreaser, a lubricant, in synthetic transformer oils, and as a solvent in chemical manufacturing. 1,2,4-Trichlorobenzene was formerly used as an insecticide against termites.

EPA Air Toxics

EPA CPDat Chemical and Product Categories

#### EPA Chemical and Products Database (CPDat)

For 1,2,4-trichlorobenzene (USEPA/OPP Pesticide Code: 081101) there are 0 labels match. /SRP: Not registered for current use in the U.S., but approved pesticide uses may change periodically and so federal, state and local authorities must be consulted for currently approved uses./

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on 1,2,4-Trichlorobenzene (120-82-1). Available from, as of July 13, 2009: https://npirspublic.ceris.purdue.edu/ppis/

#### Hazardous Substances Data Bank (HSDB)

#### Solvent in chemical manufacturing, dyes and intermediates, dielectric fluid, synthetic transformer oils, lubricants, heat-transfer medium, insecticides.

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1265

Hazardous Substances Data Bank (HSDB)

# Trichlorobenzene ... has been used as a soil treatment to repel or poison termites around the foundation of buildings. The technical product is a mixture of the 1,2,3- and 1,2,4- isomers. /SRP: Former use/

Ullmann's Encyclopedia of Industrial Chemistry. 6th ed.Vol 1: Federal Republic of Germany: Wiley-VCH Verlag GmbH & Co. 2003 to Present, p. V18 208

Hazardous Substances Data Bank (HSDB)

#### Used as a comonomer with p-dichlorobenzene in the production of arylene sulfide polymers.

Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V18 812 (1982)

Hazardous Substances Data Bank (HSDB)

For more Uses (Complete) data for 1,2,4-TRICHLOROBENZENE (6 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

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#### 8.2.1 Industry Uses

Functional fluids (closed systems)	
Intermediates	
Laboratory chemicals	
ag chemical pesticide	
https://www.epa.gov/chemical-data-reporting	

EPA Chemicals under the TSCA

#### 8.2.2 Consumer Uses

Non-TSCA use

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

EPA Chemicals under the TSCA

#### 8.3 Methods of Manufacturing

The batch reaction of benzene with a 2.8-fold molar quantity of chlorine in the presence of ferric chloride at temperatures increasing to 100 °C gives a chlorination mixture consisting of 26% 1,4-dichlorobenzene, 4.5% 1,2-dichlorobenzene, 48% 1,2,4trichlorobenzene, 8% 1,2,3-trichlorobenzene, 8% 1,2,3,4-tetrachlorobenzene, 5.5% 1,2,4,5-tetrachlorobenzene, and less than 1% pentachlorobenzene. The proportion of 1,4-dichlorobenzene, and thus also of 1,2,4-trichlorobenzene, can be raised by adding sulfur compounds as cocatalysts. After the chlorination mixture has been neutralized it can be separated by fractional distillation provided a column with more than 60 practical plates is used.

Ullmann's Encyclopedia of Industrial Chemistry. 6th ed.Vol 1: Federal Republic of Germany: Wiley-VCH Verlag GmbH & Co. 2003 to Present, p. V8 113 (2003)

#### Hazardous Substances Data Bank (HSDB)

... Production method applicable to 1,2,4- and 1,2,3-trichlorobenzenes is based on the dehydrohalogenation of 1,2,3,4,5,6-hexachlorocyclohexane (stereoisomeric mixture), a byproduct of gamma-hexachlorocyclohexane production. In the presence of aqueous alkali or alkaline earth solutions or of ammonia, or directly through use of catalysts, hexachlorocyclohexane is converted at a temperature of 90 - 250 °C mainly to trichlorobenzene. The yield lies between 80 and 99%, with the product mixture consisting of 70 - 85% 1,2,4-trichlorobenzene and 13 - 30% 1,2,3-trichlorobenzene.

Ullmann's Encyclopedia of Industrial Chemistry. 6th ed. Vol 1: Federal Republic of Germany: Wiley-VCH Verlag GmbH & Co. 2003 to Present, p. V8 113 (2003)

Hazardous Substances Data Bank (HSDB)

#### Chlorination of monochlorobenzene

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1265

Hazardous Substances Data Bank (HSDB)

... From 2,4-dichloroaniline or 2,5-dichloroaniline or 3,4-dichloroaniline by diazotization and treatment with Cu2Cl2. ... From 1,3-diaminobenzene by tetrazotization & treatment with Cu2Cl2.

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1655

Hazardous Substances Data Bank (HSDB)

#### Dehydrochlorination at 60 °C of the alpha, delta, and gamma isomers of benzene hexachloride.

Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V5 812 (1979)

Hazardous Substances Data Bank (HSDB)

#### 8.4 Formulations/Preparations

Grades: Technical; 99%; mixture of 1,2,4- and 1,2,3-isomers distilling at 213-219 °C

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1265

#### Hazardous Substances Data Bank (HSDB)

## 8.5 U.S. Production

## Aggregated Product Volume (EPA CDR 2016)

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

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

EPA Chemicals under the TSCA

(1972) 7.10X10+9 g

SRI

Hazardous Substances Data Bank (HSDB)

(1973) 1.28X10+10 g

SRI

Hazardous Substances Data Bank (HSDB)

(1982) 2,750,000 to 8,070,000 lb/yr 51 FR 11729 (4/7/86)

Hazardous Substances Data Bank (HSDB)

Benzene, 1,2,4-trichloro- is listed as a High Production Volume (HPV) chemical (65FR81686). Chemicals listed as HPV were produced in or imported into the U.S. in >1 million pounds in 1990 and/or 1994. The HPV list is based on the 1990 Inventory Update Rule. (IUR) (40 CFR part 710 subpart B; 51FR21438).

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program. Benzene, 1,2,4-trichloro- (120-82-1). Available from, as of July 13, 2009: https://www.epa.gov/hpv/pubs/general/opptsrch.htm

#### Hazardous Substances Data Bank (HSDB)

For more U.S. Production (Complete) data for 1,2,4-TRICHLOROBENZENE (6 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

8.6 U.S. Imports	0 2
(1975) 8.78X10+8 g (Principle Customs Distributors)	
SRI	
Hazardous Substances Data Bank (HSDB)	
(1983) 1.39X10+9 g /1,2,3- and 1,2,4-Trichlorobenzene/	
USITC. Imports of Benzenoid Chem & Prod: 29 (1983)	

Hazardous Substances Data Bank (HSDB)

#### 8.7 General Manufacturing Information

# Industry Processing Sectors Pesticide, fertilizer, and other agricultural chemical manufacturing Pharmaceutical and medicine manufacturing

Services Wholesale and retail trade

EPA Chemicals under the TSCA

#### **EPA TSCA Commercial Activity Status**

Benzene, 1,2,4-trichloro-: ACTIVE

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

EPA Chemicals under the TSCA

1,2,4-Trichlorobenzene is formed in minor quantities during the production of monochlorobenzene.

Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present, p. VA6 337

Hazardous Substances Data Bank (HSDB)

#### 8.8 Sampling Procedures

NIOSH Method 5517. Analyte: 1,2,4-trichlorobenzene. Matrix: Air. Sampler: Filter and solid sorbent tube (PTT-E fiber mat + Amberlite XAD-2, 100 mg/50 mg). Flow Rate: 0.01 to 0.2 l/min. Sample Size: 10 liters. Shipment: Separate filter and sorbent tube. Sample Stability: No significant losses after 13 d @ room temperature.

U.S. Department of Health and Human Services, Public Health Service. Centers for Disease Control, National Institute for Occupational Safety and Health. NIOSH Manual of Analytical Methods, 3rd ed. Volumes 1 and 2 with 1985 supplement, and revisions. Washington, DC: U.S. Government Printing Office, February 1984., p. V2 5517-1

#### Hazardous Substances Data Bank (HSDB)

Air Samples: ... An air sampling tube packed with two sections of Amberlite XAD-2 resin separated by a silanized glass wool plug, to collect the chlorobenzenes /is used/. The adsorbent is desorbed with carbon tetrachloride. /Chlorobenzenes/

Langhorst ML, Nestrick TJ; Anal Chem 51 (12): 2018-25 as cited in USEPA; Health Assessment Document: Chlorinated Benzenes p.3-17 EPA 600/8-84-015

#### Hazardous Substances Data Bank (HSDB)

A SIMPLIFIED QUANTITATIVE METHOD IS DESCRIBED FOR COLLECTION OF AIR POLLUTANTS ON A POROUS POLYMER (TENAX GC) TRAP. ... THE METHOD WAS APPLIED TO A NUMBER OF VOLATILE INDUSTRIAL SUBSTANCES FROM STACKS & AMBIENT AIR SUCH AS CHLORO COMPOUNDS WHICH INCL TRICHLOROBENZENE. /TRICHLOROBENZENE/

PARSONS JS, MITZNER S; ENVIRON SCI TECHNOL 9 (12): 1053-8 (1975)

Hazardous Substances Data Bank (HSDB)

9 Identification	? Z
9.1 Analytic Laboratory Methods	0 2
Method: EPA 8121; Procedure: gas chromatography; Analyte: 1,2,4-trichlorobenzene; Matrix: environmental samples and RCRA wastes; Detection Limit: 130 nanogram/L. U.S. Environmental Protection Agency. Solid Waste Test Methods SW-846 with Update III. CD-ROM (ISO 9660, V381SW8). Solutions Software Corp (1998) Hazardous Substances Data Bank (HSDB)	
Method: NIOSH 5517, Issue 2; Procedure: gas chromatography, (63)Ni electron capture detector; Analyte: 1,2,4-trichlorobenzene; Matrix: air; Detection Limit: 0.001 ug/mL in hexane. CDC; NIOSH Manual of Analytical Methods, 4th ed. 1,2,4-Trichlorobenzene (120-82-1). Available from, as of July 17, 2009; https://www.cdc.gov/niosh/docs/2003-154/	
Hazardous Substances Data Bank (HSDB)	
Method: ASTM D5790; Procedure: gas chromatography/mass spectrometry; Analyte: 1,2,4-trichlorobenzene; Matrix: validated for treated drinking water, wastewater, and ground water; Detection Limit: 0.21 ug/L. National Environmental Methods Index; Analytical, Test and Sampling Methods. 1,2,4-Trichlorobenzene (120-82-1). Available from, as of July 16, 2009: https://www.nemi.gov	
Hazardous Substances Data Bank (HSDB)	
Method: DOE OM100R; Procedure: gas chromatography/mass spectrometry; Analyte: 1,2,4-trichlorobenzene; Matrix: solid waste matrices, soils, and groundwater; Detection Limit: 34 ug/L. National Environmental Methods Index; Analytical, Test and Sampling Methods. 1,2,4-Trichlorobenzene (120-82-1). Available from, as of July 16, 2009: https://www.nemi.gov	
Hazardous Substances Data Bank (HSDB)	
For more Analytic Laboratory Methods (Complete) data for 1,2,4-TRICHLOROBENZENE (32 total), please visit the HSDB record page.	
Hazardous Substances Data Bank (HSDB)	
9.2 Clinical Laboratory Methods	0 Z
Complex sample matrixes of estuarine biota tissue were analyzed for selected chlorinated cmpd /including 1,2,4-trichlorobenzene/ using GC /positive chemical ionization/tandem MS. The detection limit was 20 pg, and the instrument orders of magnitude.	response was linear over 5
Rostad CE, Pereira WE; Biomed Environ Mass Spectrom 18 (7): 464-70 (1989)	
Hazardous Substances Data Bank (HSDB)	
The detection of chlorinated aromatic hydrocarbons (o-, m-, p-dichlorobenzene; 1,2,4-trichlorobenzene; 1,2,4,5-tetrachlorobenzene; pentachlorobenzene; hexachlorobenzene) in human blood plasma by capillary gas chromatography Lewalter J, Elirich D; Anal Hazard Subst Biol Mater 3: 93-108 (1991)	is described and discussed.
Hazardous Substances Data Bank (HSDB)	
9.3 OSHA Chemical Sampling	0 Z
GC - NIOSH 5517 (fully validated)	
Occupational Safety and Health Administration (OSHA)	

9.4 NIOSH Analytical Methods	

#### POLYCHLOROBENZENES 5517

NIOSH Manual of Analytical Methods

10 Safety and Hazards	0 🛛
0.1 Hazards Identification	0 Z
0.1.1 GHS Classification	? Z

# Showing 1 of 5 View More

Pictogram(s)	kritant Hazard
Signal	Warning
GHS Hazard Statements	H302: Harmful if swallowed [Warning Acute toxicity, oral] H315: Causes skin irritation [Warning Skin corrosion/irritation] H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard] H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P264, P270, P273, P280, P301+P312, P302+P352, P321, P330, P332+P313, P362, P391, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

#### EU REGULATION (EC) No 1272/2008

10.1.2 Hazard Classes and Categories	
Showing 2 of 5 View More	
Acute Tox. 4 *	
Skin Irrit. 2	
Aquatic Acute 1	
Aquatic Chronic 1	
► EU REGULATION (EC) No 1272/2008	
Acute Tox. 4 (100%)	
Skin Irrit. 2 (98.73%)	
Acute Tox. 3 (44.3%)	
Aquatic Acute 1 (97.47%)	
Aquatic Chronic 1 (100%)	
European Chemicals Agency (ECHA)	

10.1.3 NFPA Hazard C	Classification	? Z
Showing 1 of 2 View More		
NFPA 704 Diamond	2-1-0	
NFPA Health Rating	2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.	
NFPA Fire Rating	1 - Materials that must be preheated before ignition can occur. Materials require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur.	
NFPA Instability Rating	0 - Materials that in themselves are normally stable, even under fire conditions.	

Hazardous Substances Data Bank (HSDB)

#### 10.1.4 Health Hazards

Exposures to high concentrations via inhalation are potentially hazardous to the lungs, kidneys and liver. Prolonged or repeated exposures or short exposure to high concentrations via inhalation are potentially hazardous to the lungs, kidneys and liver. Prolonged or repeated exposures to short exposure to high concentrations via inhalation are potentially hazardous to the lungs, kidneys and liver. Prolonged or repeated exposure to the eyes is likely to result in moderate pain and transient irritation. Prolonged or repeated contact with the skin may result in moderate irritation and possible systemic effects. Ingestion: May cause kidney and liver damage. (USC G, 1999) U.S. Coast Guard. 1999. Chemical Hazard Response Information System (CHRIS) - Hazardous Chemical Data. Commandant Instruction 16465.12C. Washington, D.C.: U.S. Government Printing Office.

#### CAMEO Chemicals

#### 10.1.5 Fire Hazards

Special Hazards of Combustion Products: May contain toxic hydrogen chloride and phosgene. Behavior in Fire: Decomposes to form hydrogen chloride and phosgene. (USCG, 1999)

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

CAMEO Chemicals

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

ILO International Chemical Safety Cards (ICSC)

#### 10.1.6 Hazards Summary

Occupational exposure to 1,2,4-trichlorobenzene may occur from inhalation during its manufacture and use. No information is available on the acute (short-term), reproductive, developmental, and carcinogenic effects of 1,2,4-trichlorobenzene in humans. Local irritation of the lungs and dyspnea have been reported in animals following acute inhalation exposure. Chronic oral exposure has been observed to result in increased adrenal weights and vacuolization of the zona fasciculata in the cortex in rats. Liver effects have also been reported following chronic oral exposure in rats. EPA has classified 1,2,4-trichlorobenzene as a Group D, not classifiable as to human carcinogenicity.

EPA Air Toxics

#### 10.1.7 Fire Potential

#### Vapor explosion hazard indoors, outdoors, or in sewers. Runoff to sewer may creat fire or explosion hazard.

Sittig, M. Handbook of Toxic and Hazardous Chemicals and Carcinogens, 2002. 4th ed. Vol 1 A-H Norwich, NY: Noyes Publications, 2002., p. 2245

Hazardous Substances Data Bank (HSDB)

#### Combustible when exposed to heat or flame.

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 3231

Hazardous Substances Data Bank (HSDB)

#### 10.1.8 Skin, Eye, and Respiratory Irritations

Skin: may cause severe irritation. Prolonged contact may cause skin burns. Eyes: Causes irritation. Levels greater than 5 ppm may cause severe irritation.

Sittig, M. Handbook of Toxic and Hazardous Chemicals and Carcinogens, 2002. 4th ed.Vol 1 A-H Norwich, NY: Noyes Publications, 2002., p. 2243

Hazardous Substances Data Bank (HSDB)

#### Industrial data report ... minimal eye & throat irritation at 3-5 ppm in certain people.

American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values and Biological Exposure Indices. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991., p. 1605

Hazardous Substances Data Bank (HSDB)

#### Solid 1,2,4-trichlorobenzene ... is irritating & causes severe pain on contact with eyes.

Grant, W.M. Toxicology of the Eye. 3rd ed. Springfield, IL: Charles C. Thomas Publisher, 1986., p. 934

Hazardous Substances Data Bank (HSDB)

#### Chlorinated benzenes are irritating to the skin, conjunctiva, and mucous membranes of the upper respiratory tract. ... /Chlorinated benzenes/

Sittig, M. Handbook of Toxic and Hazardous Chemicals and Carcinogens, 1985. 2nd ed. Park Ridge, NJ: Noyes Data Corporation, 1985., p. 879

Hazardous Substances Data Bank (HSDB)

#### https://pubchem.ncbi.nlm.nih.gov/compound/13#section=Safety-and-Hazards

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10.2.1 Flammable Limits	) []

Lower Flammable Limit: 2.5% by vol at 302 °F (150 °C). Upper Flammable Limit: 6.6% by vol at 302 °F (150 °C)

Fire Protection Guide to Hazardous Materials. 13 ed. Quincy, MA: National Fire Protection Association, 2002., p. 325-109

#### Hazardous Substances Data Bank (HSDB)

#### Flammability

Class IIIB Combustible Liquid: FI.P. at or above 200°F.

#### Combustible Solid

The National Institute for Occupational Safety and Health (NIOSH)

#### 10.2.2 Lower Explosive Limit (LEL)

#### 2.5 % at 302° 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

#### 2.5% at 302°F

Occupational Safety and Health Administration (OSHA)

#### (302°F): 2.5%

The National Institute for Occupational Safety and Health (NIOSH)

10.2.3 Upper Explosive Limit (UEL)	2 C
6.6 % at 302° 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	
6.6% at 302°F	
Occupational Safety and Health Administration (OSHA)	
10.2.4 Critical Temperature & Pressure	0 Z
Critical temperature: 453.3 °C; critical pressure: 3718 kPa Krishnamurti R; Kirk-Othmer Encyclopedia of Chemical Technology. (2001). NY, NY: John Wiley & Sons; Chlorinated Benzenes. Online Posting Date: Jul 13, 2001.	
Hazardous Substances Data Bank (HSDB)	
10.2.5 Explosive Limits and Potential	0 2

#### Explosive limits 2.5-6.6 % vol (at 150 °C)

NIOSH; International Chemical Safety Card on 1,2,4-Trichlorobenzene (ICSC # 1049) (November 2003). Available from, as of July 17, 2009: https://www.cdc.gov/niosh/ipcsneng/neng1049.html

Hazardous Substances Data Bank (HSDB)

#### Explosive limits , vol% in air: 2.5-6.6 (at 150 °C)

ILO International Chemical Safety Cards (ICSC)

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#### 10.2.6 OSHA Standards

Vacated 1989 OSHA PEL Ceiling limit 5 ppm (40 mg/cu m) is still enforced in some states.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 372

Hazardous Substances Data Bank (HSDB)

10.2.7 NIOSH Recommendations	0 2

#### Recommended Exposure Limit: Ceiling value: 5 ppm (40 mg/cu m).

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases CD-ROM. Department of Health & Human Services, Centers for Disease Prevention & Control. National Institute for Occupational Safety & Health. DHHS (NIOSH) Publication No. 2005-151 (2005)

Hazardous Substances Data Bank (HSDB)

10.3 First Aid Measures	? Z
10.3.1 First Aid	0 Z

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. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment. 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 rescueres entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing. INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is conscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital if advised by 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

#### (See procedures)

Eye:Irrigate immediately - If this chemical contacts the eyes, immediately wash (irrigate) the eyes with large amounts of water, occasionally lifting the lower and upper lids. Get medical attention immediately.

Skin:Soap wash - If this chemical contacts the skin, wash the contaminated skin with soap and water.

Breathing:Respiratory support

Swallow:Medical attention immediately - If this chemical has been swallowed, get medical attention immediately.

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

10.3.2 Inhalation First Aid	0 2
Fresh air, rest. Refer for medical attention.	
ILO International Chemical Safety Cards (ICSC)	
10.3.3 Skin First Aid	0 2
Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .	
ILO International Chemical Safety Cards (ICSC)	
10.3.4 Eye First Aid	0 2

#### 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)

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Rinse mouth. Give one or two glasses of water to drink. Refer for medical attention

ILO International Chemical Safety Cards (ICSC)

# 10.4 Fire Fighting

Fire Extinguishing Agents: Small fires: dry chemical, CO 2, water spray or foam; large fires: water spray, fog or foam. (USCG, 1999)

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

CAMEO Chemicals

10.3.5 Ingestion First Aid

#### Use water spray, powder, foam, carbon dioxide.

ILO International Chemical Safety Cards (ICSC)

# 10.4.1 Fire Fighting Procedures

Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Solid streams of water may spread fire. Cool all affected containers with flooding quantities of water from as far a distance as possible. Use foam, dry chemical, or carbon dioxide.

Association of American Railroads; Bureau of Explosives. Emergency Handling of Hazardous Materials in Surface Transportation. Association of American Railroads, Pueblo, CO. 2005, p. 901

#### Hazardous Substances Data Bank (HSDB)

10.5 Accidental Release Measures	?∠
10.5.1 Isolation and Evacuation	⊘ ℤ

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 Transport of 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

#### 10.5.2 Spillage Disposal

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

ILO International Chemical Safety Cards (ICSC)

#### 10.5.3 Cleanup Methods

SRP: Wastewater from contaminant suppression, cleaning of protective clothing/equipment, or contaminated sites should be contained and evaluated for subject chemical or decomposition product concentrations. Concentrations shall be lower than applicable environmental discharge or disposal criteria. Alternatively, pretreatment and/or discharge to a POTW is acceptable only after review by the governing authority. Due consideration shall be given to remediation worker exposure (inhalation, dermal and ingestion) as well as fate during treatment, transfer and disposal. If it is not practicable to manage the chemical in this fashion, it must meet Hazardous Material Criteria for disposal.

Hazardous Substances Data Bank (HSDB)

If material or contaminated runoff enters waterways, notify downstream users of potentially contaminated waters. Notify local health and fire officials and pollution control agencies.

Sittig, M. Handbook of Toxic and Hazardous Chemicals and Carcinogens, 2002. 4th ed. Vol 1 A-H Norwich, NY: Noyes Publications, 2002., p. 2244

Hazardous Substances Data Bank (HSDB)

Absorb the spills with paper towels or like materials. Place in a hood to evaporate. Dispose by burning the towel.

ITII. Toxic and Hazardous Industrial Chemicals Safety Manual. Tokyo, Japan: The International Technical Information Institute, 1988., p. 535

Hazardous Substances Data Bank (HSDB)

#### https://pubchem.ncbi.nlm.nih.gov/compound/13#section=Safety-and-Hazards

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## 10.5.4 Disposal Methods

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

Hazardous Substances Data Bank (HSDB)

Land spill. Dig a pit, pond, lagoon, holding area to contain liquid or solid material. /SRP: If time permits, pits, ponds, lagoons, soak holes, or holding areas should be sealed with an impermeable flexible membrane liner./Dike surface flow using soil, sand bags, foamed polyurethane, or foamed concrete. Absorb bulk liquid with fly ash, cement powder, or commercial sorbents. Apply universal gelling agent to immobilize spill. Apply appropriate foam to diminish vapor and fire hazard. Water spill. Use natural deep water pockets, excavated lagoons, or sand bag barriers to trap material at bottom. If dissolved, in region of 10 ppm or greater concentration, apply activated carbon at ten times the spilled amount. Remove trapped material with suction hoses. Use mechanical dredges or lifts to remove immobilized masses of pollutants and precipitates. Air spill. Apply water spray or mist to knock down vapors. Combustion products include corrosive or toxic vapors.

Association of American Railroads; Bureau of Explosives. Emergency Handling of Hazardous Materials in Surface Transportation. Association of American Railroads; Pueblo, CO. 2005, p. 901-2

#### Hazardous Substances Data Bank (HSDB)

Incineration, preferably after mixing with another combustible fuel. Care must be exercised to assure complete combustion to prevent the formation of phosgene. An alkali scrubber is necessary to remove the halo acids produced. Recommendable method: Incineration.

United Nations. Treatment and Disposal Methods for Waste Chemicals (IRPTC File). Data Profile Series No. 5. Geneva, Switzerland: United Nations Environmental Programme, Dec. 1985., p. 105

#### Hazardous Substances Data Bank (HSDB)

In the powdered activated carbon treatment (PACT) process, powdered activated carbon is used with the activated sludge method for wastewater treatment. Primary treatment consists of neutralization with lime and settling followed by combined powdered activated carbon-activated sludge for secondary/tertiary treatment. Primary sludge consisting of metal salts and unreacted lime is dewatered before disposal in a lined landfill. Powdered activated carbon and return powdered activated carbon treatment sludge are added to the primary effluent as it is fed to aeration tanks. Treated effluent is discharged after first passing through a settling lagoon. Consistency and efficiency of removal varies greatly among cmpd reported and ranges from 44% for 1,2-dichlorobenzene to 99% for a number of volatile organic compounds. For 1,2,4-trichlorobenzene, 66% was removed giving an average powdered activated carbon treatment effluent of 169 ppb.

Hutton DG; Chem Water Reuse 2: 403-28 (1981)

## Hazardous Substances Data Bank (HSDB)

The following wastewater treatment technologies have been investigated for 1,2,4-trichlorobenzene: biological treatment, stripping, solvent extraction, activated carbon, and resin adsorption. USEPA: Management of Hazardous Waste Leachate, EPA Contract No.68-03-2766 p.E-3-E-22 (1982)

Hazardous Substances Data Bank (HSDB)

## 10.5.5 Preventive Measures

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

#### Hazardous Substances Data Bank (HSDB)

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

#### Hazardous Substances Data Bank (HSDB)

Keep sparks, flames, and other sources of ignition away. Keep material out of water sources and sewers. Build dikes to contain flow as necessary. Attempt to stop leak if without undue personnel hazard. Use water spray to knock-down vapors. ... Avoid breathing vapors. Keep upwind. ... Do not handle broken packages unless wearing appropriate personal protective equipment. Wash away any material which may have contacted the body with copious amounts of water or soap and water.

Association of American Railroads; Bureau of Explosives. Emergency Handling of Hazardous Materials in Surface Transportation. Association of American Railroads, Pueblo, CO. 2005, p. 901

## Hazardous Substances Data Bank (HSDB)

#### The worker should immediately wash the skin when it becomes contaminated.

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases CD-ROM. Department of Health & Human Services, Centers for Disease Prevention & Control. National Institute for Occupational Safety & Health. DHHS (NIOSH) Publication No. 2005-151 (2005)

## Hazardous Substances Data Bank (HSDB)

## Work clothing that becomes wet or significantly contaminated should be removed and replaced.

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases CD-ROM. Department of Health & Human Services, Centers for Disease Prevention & Control. National Institute for Occupational Safety & Health. DHHS (NIOSH) Publication No. 2005-151 (2005)

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Hazardous Substances Data Bank (HSDB)

10.6 Handling and Storage	0 2
10.6.1 Nonfire Spill Response	0 2

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 keep it away from oxidizing materials. (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

10.6.2 Safe Storage	0 Z
Separated from strong oxidants, acids and food and feedstuffs.	
ILO International Chemical Safety Cards (ICSC)	

## 10.6.3 Storage Conditions

1,2,4-Trichlorobenzenes are liquids at room temperature and are shipped in bulk in aluminum tank trucks and steel or stainless steel tank cars.

Kirk-Othmer Encyclopedia of Chemical Technology. 5th ed. Volumes 1: New York, NY. John Wiley and Sons, 2001-Present.

## Hazardous Substances Data Bank (HSDB)

1,2,4-Trichlorobenzene must be stored to avoid contact with oxidizers (such as perchlorates, peroxides, permanganates, chlorates and nitrates) since violent reactions occur. Sources of ignition, such as smoking and open flames, are prohibited where 1,2,4-trichlorobenzene is used, handled, or stored in a manner that could create a potential fire or explosion hazard.

Sittig, M. Handbook of Toxic and Hazardous Chemicals and Carcinogens, 2002. 4th ed.Vol 1 A-H Norwich, NY: Noyes Publications, 2002., p. 2243

Hazardous Substances Data Bank (HSDB)

10.7 Exposure Control and Personal Protection	02
10.7.1 Recommended Exposure Limit (REL)	0 Z

## REL-C (Ceiling)

5 ppm (40 mg/m<sup>3</sup>)

Occupational Safety and Health Administration (OSHA)

## C 5 ppm (40 mg/m<sup>3</sup>)

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

10.7.2 Permissible Exposure Limit (PEL)	() Z
CAPEL-C (California PEL - Ceiling)	
5 ppm (40 mg/m³)	

Occupational Safety and Health Administration (OSHA)

## none See Appendix G

10.7.3 Immediately Dangerous to Life or Health (IDLH)

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## N.D.

#### See: IDLH INDEX

The National Institute for Occupational Safety and Health (NIOSH)

## 10.7.4 Threshold Limit Values (TLV)

#### Ceiling Limit: 5 ppm

American Conference of Governmental Industrial Hygienists. Threshold Limit Values of Chemical Substances and Biological Exposure Indices, ACGIH, Cincinnati, OH 2009, p. 58

## Hazardous Substances Data Bank (HSDB)

## 5 ppm as STEL.

ILO International Chemical Safety Cards (ICSC)

skin absorption (H); carcinogen category: 3.

ILO International Chemical Safety Cards (ICSC)

## TLV-C (Ceiling)

5 ppm [1975]

Occupational Safety and Health Administration (OSHA)

10.7.5 Other Standards Regulations and Guidelines	? Z
Australia: peak limitation 5 ppm; Federal Republic of Germany: 5 ppm, short-term level 50 ppm, 30 minutes, once per shift, pregnancy Group D, data insufficient for final evaluation; United Kingdom: 5 ppm, 10-minute STEL 5 ppm. American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values and Biological Exposure Indices. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991., p. 1606	
Hazardous Substances Data Bank (HSDB)	
10.7.6 Inhalation Risk	?∠
A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20 °C; on spraying or dispersing, however, much faster.	
ILO International Chemical Safety Cards (ICSC)	
10.7.7 Effects of Short Term Exposure	? ⊿
The substance is irritating to the eyes, skin and respiratory tract.	
ILO International Chemical Safety Cards (ICSC)	
10.7.8 Effects of Long Term Exposure	0 Z
The substance defats the skin, which may cause dryness or cracking. The substance may have effects on the liver.	
ILO International Chemical Safety Cards (ICSC)	
10.7.9 Personal Protective Equipment (PPE)	⊘ ⊿

Skin: Wear appropriate personal protective clothing to prevent skin contact. Eyes: Wear appropriate eye protection to prevent eye contact. Wash skin: The worker should immediately wash the skin when it becomes contaminated. Remove: Work clothing that becomes wet or significantly contaminated should be removed and replaced. Change: No recommendation is made specifying the need for the worker to change clothing after the work shift. (NIOSH, 2016)

National Institute of Occupational Safety and Health. NIOSH Pocket Guide to Chemical Hazards (full website version). https://www.cdc.gov/niosh/npg (accessed August 2016).

CAMEO Chemicals

## Wear appropriate chemical protective gloves, boots and goggles. Wear positive pressure self-contained breathing apparatus when fighting fires involving this material.

Association of American Railroads; Bureau of Explosives. Emergency Handling of Hazardous Materials in Surface Transportation. Association of American Railroads, Pueblo, CO. 2005, p. 901

Hazardous Substances Data Bank (HSDB)

## Wear appropriate personal protective clothing to prevent skin contact.

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases CD-ROM. Department of Health & Human Services, Centers for Disease Prevention & Control. National Institute for Occupational Safety & Health. DHHS (NIOSH) Publication No. 2005-151 (2005)

Hazardous Substances Data Bank (HSDB)

## Wear appropriate eye protection to prevent eye contact.

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases CD-ROM. Department of Health & Human Services, Centers for Disease Prevention & Control. National Institute for Occupational Safety & Health. DHHS (NIOSH) Publication No. 2005-151 (2005)

#### Hazardous Substances Data Bank (HSDB)

## (See protection codes)

Skin:Prevent skin contact - Wear appropriate personal protective clothing to prevent skin contact.

Eyes:Prevent eye contact - Wear appropriate eye protection to prevent eye contact.

Wash skin:When contaminated

Remove:When wet or contaminated

Change:No recommendation

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

10.7.10 Respirator Recommendations	(?) [ <sup>'</sup> ]
Important additional information about respirator selection	
The National Institute for Occupational Safety and Health (NIOSH)	
10.7.11 Fire Prevention	0 2
NO open flames.	
ILO International Chemical Safety Cards (ICSC)	
10.7.12 Exposure Prevention	0 Z
PREVENT GENERATION OF MISTS!	
ILO International Chemical Safety Cards (ICSC)	
10.7.13 Inhalation Prevention	0 2
Use ventilation, local exhaust or breathing protection.	
ILO International Chemical Safety Cards (ICSC)	
10.7.14 Skin Prevention	0 2
Protective gloves.	
ILO International Chemical Safety Cards (ICSC)	
10.7.15 Eye Prevention	0 Z
Wear safety goggles or eye protection in combination with breathing protection.	

https://pubchem.ncbi.nlm.nih.gov/compound/13#section=Safety-and-Hazards

►	ILO International Chemical Safety Cards (ICSC)
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10.7.16 Ingestion Prevention	0 Z
Do not eat, drink, or smoke during work.	
ILO International Chemical Safety Cards (ICSC)	
	-
10.8 Stability and Reactivity	0 2
10.8.1 Air and Water Reactions	0 Z
Insoluble in water.	
CAMEO Chemicals	
10.8.2 Reactive Group	0 Z
Aryl Halides	
CAMEO Chemicals	
	0.55
10.8.3 Reactivity Profile	? 🛽
1,2,4-TRICHLOROBENZENE can react vigorously with oxidizing materials (NTP, 1992). Yields hydrogen chloride and phosgene when heated to decomposition (USCG, 1999).	
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.	
10.8.4 Hazardous Reactivities and Incompatibilities	0 Z
On contact with acids or acid fumes they evolve highly toxic /hydrogen chloride/ fumes. /chlorides/	
Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 715	
Hazardous Substances Data Bank (HSDB)	
Can react vigorously with oxidizing materials.	
Lewis, RJ. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 3231	
Hazardous Substances Data Bank (HSDB)	
Acids, acid fumes, oxidizers, steam.	
NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases CD-ROM. Department of Health & Human Services, Centers for Disease Prevention & Control. National Institute for Occupational Safety & Health. DHHS (NIOSH) Publication No. 2005-151 (2005)	
Hazardous Substances Data Bank (HSDB)	
10.9 Transport Information	0 Z
10.9.1 DOT Emergency Guidelines	0 Z
/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 e	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. /Trichlorobenzenes, liquid/	-,,,,
U.S. Department of Transportation. 2008 Emergency Response Guidebook. Washington, D.C. 2008	

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. ... 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. /Trichlorobenzenes, liquid/

## 1,2,4-Trichlorobenzene | C6H3Cl3 - PubChem

U.S. Department of Transportation. 2008 Emergency Response Guidebook. Washington, D.C. 2008

## 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 m (150 ft) for liquids and at least 25 m (75 ft) for solids. Keep unauthorized personnel away. Stay upwind. Keep out of low areas. Ventilate enclosed areas. /Trichlorobenzenes, liquid/

U.S. Department of Transportation. 2008 Emergency Response Guidebook. Washington, D.C. 2008

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. /Trichlorobenzenes, liquid/

Hazardous Substances Data Bank (HSDB)

For more DOT Emergency Guidelines (Complete) data for 1,2,4-TRICHLOROBENZENE (8 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

10.9.2 DOT ID and Guide	
2321 153 (liquid)	
The National Institute for Occupational Safety and Health (NIOSH)	

0.9.3 Shipping Name/ Number DOT/UN/NA/IMO	0 🛛

UN 2321; Trichlorobenzenes, liquid or 1,2,4-trichlorobenzene

Hazardous Substances Data Bank (HSDB)

IMO 6.1; Trichlorobenzenes, liquid or 1,2,4-trichlorobenzene

Hazardous Substances Data Bank (HSDB)

10.9.4 Shipment Methods and Regulations	? Z

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. 39th Ed. Montreal, Canada and Geneva, Switzerland : International Air Transport Association, Dangerous Goods Regulations, 1998., p. 198

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.6241 (1988)* 

Hazardous Substances Data Bank (HSDB)

#### 10.9.5 DOT Label

Poison

CAMEO Chemicals

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10.9.6 Packaging and Labelling	0 2
Do not transport with food and feedstuffs. Marine pollutant.	
ILO International Chemical Safety Cards (ICSC)	
10.9.7 EC Classification	(?) 🛛
Symbol: Xn, N; R: 22-38-50/53; S: (2)-23-37/39-60-61	
ILO International Chemical Safety Cards (ICSC)	
10.9.8 UN Classification	(?) 🗹
UN Hazard Class: 6.1; UN Pack Group: III	
ILO International Chemical Safety Cards (ICSC)	
10.10 Regulatory Information	(?) [/
10.10.1 Atmospheric Standards	0 2

This action promulgates standards of performance for equipment leaks of Volatile Organic Compounds (VOC) in the Synthetic Organic Chemical Manufacturing Industry (SOCMI). The intended effect of these standards is to require all newly constructed, modified, and reconstructed SOCMI process units to use the best demonstrated system of continuous emission reduction for equipment leaks of VOC, considering costs, non air quality health and environmental impact and energy requirements. Trichlorobenzenes are produced, as an intermediate or final product, by process units covered under this subpart. /The standards apply to all of the isomers and mixtures./

40 CFR 60.489 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 9, 2009: https://www.ecfr.gov

Hazardous Substances Data Bank (HSDB)

Listed as a hazardous air pollutant (HAP) generally known or suspected to cause serious health problems. The Clean Air Act, as amended in 1990, directs EPA to set standards requiring major sources to sharply reduce routine emissions of toxic pollutants. EPA is required to establish and phase in specific performance based standards for all air emission sources that emit one or more of the listed pollutants. 1,2,4-Trichlorobenzene is included on this list. Clean Air Act as amended in 1990, Sect. 112 (b) (1) Public Law 101-549 Nov. 15, 1990

Hazardous Substances Data Bank (HSDB)

10.10.2 Federal Drinking Water Standards	? ℤ
EPA 70 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)	
10.10.3 Federal Drinking Water Guidelines	? Z
EPA 70 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)	
10.10.4 State Drinking Water Standards	0 Z
(CA) CALIFORNIA 5 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)

(NJ) NEW JERSEY 9 ug/L

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# 1,2,4-Trichlorobenzene | C6H3Cl3 - PubChem

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)

# $\odot$ $\square$ 10.10.5 State Drinking Water Guidelines (AZ) ARIZONA 140 ug/L USEPA/Office of Water, Federal-State Toxicology and Risk Analysis Committee (FSTRAC). Summary of State and Federal Drinking Water Standards and Guidelines (11/93) To Present Hazardous Substances Data Bank (HSDB) (ME) MAINE 70 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) $\bigcirc \mathbb{Z}$ 10.10.6 Clean Water Act Requirements Toxic pollutant designated pursuant to section 307(a)(1) of the Federal Water Pollution Control Act and is subject to effluent limitations. /Chlorinated benzenes (other than dichlorobenzenes)/ 40 CFR 401.15 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 9, 2009; https://www.ecfr.gov Hazardous Substances Data Bank (HSDB) $\bigcirc$ 10.10.7 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. The rule for determining when notification is required is stated in 40 CFR 302.4 (section IV.D.3.b). 40 CFR 302.4 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 9, 2009: https://www.ecfr.gov Hazardous Substances Data Bank (HSDB) $\bigcirc \square$

## 10.10.8 TSCA Requirements

Pursuant to section 8(d) of TSCA, EPA promulgated a model Health and Safety Data Reporting Rule. The section 8(d) model rule requires manufacturers, importers, and processors of listed chemical substances and mixtures to submit to EPA copies and lists of unpublished health and safety studies. 1,2,4-Trichlorobenzene is included on this list. Effective date 10/4/82; Sunset date: 10/4/92.

40 CFR 716.120 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 9, 2009: https://www.ecfr.gov

## Hazardous Substances Data Bank (HSDB)

10.11 Other Safety Information	? Z
10.11.1 Toxic Combustion Products	? Z

Poisonous gases including phosgene, chlorine, and hydrogen chloride are produced in fire.

Sittig, M. Handbook of Toxic and Hazardous Chemicals and Carcinogens, 2002. 4th ed. Vol 1 A-H Norwich, NY: Noyes Publications, 2002., p. 2244

Hazardous Substances Data Bank (HSDB)

## 10.11.2 Special Reports

USEPA; Ambient Water Quality Criteria Doc: Chlorinated Benzenes (1980) EPA 440/5-80-028.

Hazardous Substances Data Bank (HSDB)

European Chemicals Bureau; IUCLID Dataset, 1,2,4-Trichlorobenzene (120-82-1) (2000 CD-ROM edition) contains information on use, toxicology, and environmental effects of this chemical as supplied to the European Union by industry.

Hazardous Substances Data Bank (HSDB)

U.S. Environmental Protection Agency's Integrated Risk Information System (IRIS) on 1,2,4-Trichlorobennzene (120-82-1). [Available from the Substance File List, as of July 10, 2009: http://www.epa.gov/iris/index.html]

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Hazardous Substances Data Bank (HSDB)

11 Toxicity	02
11.1 Toxicological Information	⊘ ⊿
11.1.1 NIOSH Toxicity Data	? Z

The National Institute for Occupational Safety and Health (NIOSH)

## 11.1.2 Evidence for Carcinogenicity

Cancer Classification: Group D Not Classifiable as to Human Carcinogenicity

USEPA Office of Pesticide Programs, Health Effects Division, Science Information Management Branch: "Chemicals Evaluated for Carcinogenic Potential" (April 2006)

Hazardous Substances Data Bank (HSDB)

CLASSIFICATION: D; not classifiable as to human carcinogenicity. BASIS FOR CLASSIFICATION: A dermal exposure study in mice was found inadequate for drawing conclusions as to carcinogenicity in humans. HUMAN CARCINOGENICITY DATA: None. ANIMAL CARCINOGENICITY DATA: None. ANIMAL CARCINOGENICITY DATA: Inadequate.

U.S. Environmental Protection Agency's Integrated Risk Information System (IRIS). Summary on 1,2,4-Trichlorobenzene (120-82-1). Available from, as of March 15, 2000: https://www.epa.gov/iris/

Hazardous Substances Data Bank (HSDB)

EPA-D

Occupational Safety and Health Administration (OSHA)

.3 Health Effects

HE15 - Irritation-Eyes, Nose, Throat, Skin---Moderate

HE4 - Acute Toxicity---Short-term high risk effects

Occupational Safety and Health Administration (OSHA)

## 11.1.4 Exposure Routes

Health Effect Code(s)

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

ILO International Chemical Safety Cards (ICSC)

inhalation, skin absorption, ingestion, skin and/or eye contact

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The National Institute for Occupational Safety and Health (NIOSH)

11.1.5 Symptoms	0 2
irritation eyes, skin, mucous membrane; In Animals: liver, kidney damage; possible teratogenic effects	
The National Institute for Occupational Safety and Health (NIOSH)	
11.1.6 Inhalation Symptoms	0 2
Cough. Sore throat. Burning sensation.	
ILO International Chemical Safety Cards (ICSC)	
11.1.7 Skin Symptoms	? Z
Dry skin. Redness. Roughness.	
ILO International Chemical Safety Cards (ICSC)	
11.1.8 Eye Symptoms	0 2
Redness. Pain.	
ILO International Chemical Safety Cards (ICSC)	
11.1.9 Ingestion Symptoms	0 2
Abdominal pain. Sore throat. Vomiting.	
ILO International Chemical Safety Cards (ICSC)	
11.1.10 Target Organs	0 2
Eyes, skin, respiratory system, liver, reproductive system	
The National Institute for Occupational Safety and Health (NIOSH)	
11.1.11 Acute Effects	0 2

## 11.1.12 Interactions

ChemIDplus

# The halogenated benzenes, inducers of xenobiotic metabolism, were studied for their effects on the metabolism of malathion, malaoxon (lindane), and paraoxon and on the toxicity and lethality of these organophosphorus insecticides and parathion. One mmol/kg of 1,4-dichlorobenzene (p-dichlorobenzene), 1,2,4-trichlorobenzene, 1,2,4-tribromobenzene, or hexabromobenzene or 0.1 mmol/kg hexachlorobenzene was administered po to male mice daily for 7 days. In general, the trihalogenated benzenes increased the LD50 of all 4 insecticides 2- to 6-fold. These increases were larger than those observed with the di- or hexahalogenated isomers. The bromide-substituted benzenes were usually more active than the chlorinated ones with the exception being hexabromobenzene. There was a good correlation between their effects on lethality and increases in in vitro carboxylesterase activity with either malathion or malaoxon as the substrate. The trihalogenated benzenes decreased the inhibitory effect of malathion on cholinesterase activity in the brain and to a lesser degree in the red blood cells, but not in liver or plasma. There was also a good correlation between protection against parathion and paraoxon lethality, protection against inhibition of cholinesterase in the brain and to paraoxon by microsomal mixed-function oxidases but not by hepatic or plasma esterases. It appears that the halogenated benzenes are able to protect against organophosphorus insecticide toxicity. With malathion, increases in carboxylesterase activity may be important, and with paraoxon, increases in microsomal mixed-function oxidase dealkylation and tissue binding cannot be excluded from contributing to the protection seen.

Townsend BA, Carlson GP; Toxicol Appl Pharmacol 60 (1): 52-61 (1981)

Hazardous Substances Data Bank (HSDB)

## 11.1.13 Antidote and Emergency Treatment

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

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 209

## Hazardous Substances Data Bank (HSDB)

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

#### Hazardous Substances Data Bank (HSDB)

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 210

#### Hazardous Substances Data Bank (HSDB)

## 11.1.14 Human Toxicity Excerpts

/SIGNS AND SYMPTOMS/ Cutaneous exposure to 1,2,4-trichlorobenzene does not cause chloracne or acneform dermatitis but can cause dermal irritation which is probably attributable to its defatting action. American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values and Biological Exposure Indices. 5th ed. Cincinnati, OH: American Conference of Governmental Industrial Hygienists, 1986, p. 593

Hazardous Substances Data Bank (HSDB)

/SIGNS AND SYMPTOMS/ There is the potential for trichlorobenzene-induced hepatic toxicity in situations where exposures to high concentrations are encountered. American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values and Biological Exposure Indices. CD-ROM 2007.

Hazardous Substances Data Bank (HSDB)

#### 11.1.15 Non-Human Toxicity Excerpts

/LABORATORY ANIMALS: Acute Exposure/ The acute toxicity of a number of chlorinated benzenes, ranging from monosubstituted to pentasubstituted benzenes, was studied in rats. Toxic effects on the liver, the kidneys, and the thyroid were monitored after a single ip administration of 1, 2, or 4 mmol/kg monochlorobenzene (MCB), 1,2-dichlorobenzene (1,2-DICB), 1,4-dichlorobenzene (1,2-DICB), 1,2,4-trichlorobenzene (1,2,4-TRCB), and pentachlorobenzene (PECB). Due to its low solubility, 1,2,4,5-tetrachlorobenzene (1,2,4,5-TECB) was tested at a highest dose of 0.8 mmol/kg. 1,2-DICB and 1,2,4-TRCB produced the most severe hepatotoxic effects when compared with an equimolar dose of the other chlorinated benzenes, as determined by plasma ALT profile and histopathological changes after 72 hr. MCB was considerably less hepatotoxic. Severe degenerative damage to the kidney was only observed in a few rats treated with 1,2,4-TRCB. However, protein droplets in the tubular epithelial cells were observed at 72 hr. ACB and PECB. In the latter two groups, these protein droplets were still observed 9 days after administration. All chlorinated benzenes tested excluding MCB induced a reduction in plasma thyroxine levels. The extent of the relative binding affinities of the plasma transport protein for thyroxine, ie, transthyretin. The present study indicates that the establishment of a

## https://pubchem.ncbi.nlm.nih.gov/compound/13#section=Safety-and-Hazards

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## 1,2,4-Trichlorobenzene | C6H3Cl3 - PubChem

structure-activity relationship with regard to toxicity depends on the sensitivity of the respective target organs. In the series of (poly)chlorinated benzenes studied, ranging from mono- to pentachlorobenzene, the most severe effects on liver, kidney, and thyroid were observed for 1,2,4-substitution.

#### PMID:1949037

den Besten C et al; Toxicol Appl Pharmacol 111 (1): 69-81 (1991).

#### Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Acute Exposure/ A study of acute & subacute inhalation toxicity of ... 95% 1,2,4-isomer ... Indicated that target organs from non-lethal exposures of cats, dogs, rabbits, & guinea pigs included liver, kidney, ganglion cells of the brain, & it can irritate mucous membranes. Local pulmonary irritation of the lungs & dyspnea were noted in animals that later died after inhaling 1,2,4-1,2,4-trichlorobenzene. ... Sublethal doses admin repeatedly to guinea pigs caused liver damage. Short term (15 x 6-hr exposures at 70 & 200 ppm) inhalation studies failed to kill animals. ... Produced lethargy & retarded wt gain with no organ pathology.

American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values and Biological Exposure Indices. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991., p. 1605

#### Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Acute Exposure/ 1,2,4-Trichlorobenzene increased bile duct-pancreatic fluid flow and decreased its protein concentration 24 hr after ip treatment of rats of with 5.0 mmol/kg. The mechanism of increased bile duct-pancreatic fluid flow is not known, but it does not involve secretin or cholinergic stimulation of the pancrease, nor does it occur secondary to liver damage.

#### PMID:220753

Yang KH et al; Toxicol Appl Pharmacol 47 (3): 505-14 (1979)

#### Hazardous Substances Data Bank (HSDB)

#### /LABORATORY ANIMALS: Acute Exposure/ 1,2,4-Trichlorobenzene causes transient erythema by single painting on mouse skin, and acanthosis and hyperkeratosis (but not chloracne) by repeated application to rabbit ears.

International Labour Office. Encyclopedia of Occupational Health and Safety. Vols. 18/11. Geneva, Switzerland: International Labour Office, 1983., p. 460

#### Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Excerpts (Complete) data for 1,2,4-TRICHLOROBENZENE (45 total), please visit the HSDB record page.

## Hazardous Substances Data Bank (HSDB)

## 11.1.16 Non-Human Toxicity Values

#### LD50 Rat oral 756 mg/kg

ITII. Toxic and Hazardous Industrial Chemicals Safety Manual. Tokyo, Japan: The International Technical Information Institute, 1988., p. 535

#### Hazardous Substances Data Bank (HSDB)

## LD50 Mouse oral 766 mg/kg

ITII. Toxic and Hazardous Industrial Chemicals Safety Manual. Tokyo, Japan: The International Technical Information Institute, 1988., p. 535

#### Hazardous Substances Data Bank (HSDB)

#### LD50 Mouse ip 1223 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3522

Hazardous Substances Data Bank (HSDB)

## LD50 Rat percutaneous 6100 mg/kg

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

Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Values (Complete) data for 1,2,4-TRICHLOROBENZENE (7 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

## 11.1.17 Ecotoxicity Values

LC50; Species: Allolobophora tuberculata (Earthworm, adult) multiple environmental routes (using filter paper) 23 ug/sq cm for 48 hr (95% confidence interval: 16-32 ug/sq cm)

Neuhauser EF et al; Comp Biochem Physiol C 83 (1): 197-200 (1986) as cited in the ECOTOX database. Available from, as of June 29, 2009

Hazardous Substances Data Bank (HSDB)

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## 1,2,4-Trichlorobenzene | C6H3Cl3 - PubChem

LC50; Species: Allolobophora tuberculata (Earthworm, adult) direct application (artificial soil, 69% sand, 20% clay, pH 6.0, and 10% organic matter, 35% moisture) 251 mg/kg for 48 hr (95% confidence interval: 167-378 mg/kg)

Neuhauser EF et al; Comp Biochem Physiol C 83 (1): 197-200 (1986) as cited in the ECOTOX database. Available from, as of June 29, 2009

Hazardous Substances Data Bank (HSDB)

LC50; Species: Eisenia fetida (Earthworm, adult) multiple environmental routes (using filter paper) 27 ug/sq cm for 48 hr (95% confidence interval: 24-32 ug/sq cm)

Neuhauser EF et al; Comp Biochem Physiol C 83 (1): 197-200 (1986) as cited in the ECOTOX database. Available from, as of June 29, 2009

Hazardous Substances Data Bank (HSDB)

LC50; Species: Eisenia fetida (Earthworm, adult) direct application (artificial soil, 69% sand, 20% clay, pH 6.0, and 10% organic matter, 35% moisture) 197 mg/kg for 48 hr (95% confidence interval: 137-282 mg/kg) Neuhauser EF et al; Comp Biochem Physiol C 83 (1): 197-200 (1986) as cited in the ECOTOX database. Available from, as of June 29, 2009

Hazardous Substances Data Bank (HSDB)

For more Ecotoxicity Values (Complete) data for 1,2,4-TRICHLOROBENZENE (41 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

#### 11.1.18 Ecotoxicity Excerpts

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/AQUATIC SPECIES/ For ... 1,2,4-trichlorobenzene (TCBz), lethal body burdens (LBB) of ... 14 +/- 4.5 mmol/kg (ww) ... were determined in fathead minnow (Pimephales promelas). LBBs ... were found to increase with increasing lipid content and time-to-death of fish within the same aquarium. The correlation with time-to-death suggests that besides lipid content at least one other factor causes intraspecies variation in LBBs. When intraspecies variation is excluded by comparing mean LBBs from different aquaria and exposure regimes, LBBs still vary with time-to-death. In contrast to the situation within one aquarium, between different aquaria and exposure regimes often a decrease in LBB with time-to-death is found ...

## PMID:9469874

de Maagd PG et al; Ecotox Environ Safety 38 (3): 232-7 (1997).

#### Hazardous Substances Data Bank (HSDB)

/AQUATIC SPECIES/ The effects and fate of 1,2,4-trichlorobenzene were studied in fish. The high levels of biotransformation products found in rainbow trout (Salmo gardneri) bile during & after exposure in these studies support the possible use of bile sampling in pollutant-modeling programs.

USEPA; Uptake Metabolism and Disposal of Xenobiotic Chemicals in Fish p. 1-157 (1980) EPA 600/3-80-082

#### Hazardous Substances Data Bank (HSDB)

/AQUATIC SPECIES/ The cytotoxicity of 12 chem to rainbow trout (Salmo gairdneri) cells (RTG-2) was determined in culture. The indicator of cytotoxicity was the inability of cells to attach to a growth surface after chem exposure. From most toxic to least toxic, these chem were **pentachlorophenol**, **p-methylaminophenol**, **2,4-dichlorophenol**, **p-chlorophenol**, **p-cyanophenol**, **p-nitrophenol**, **benzene**, **p-methylphenol**, **aniline**, **phenol**, **p-methoxyphenol**, and 1,2,4-trichlorobenzene. The cytotoxicity of these cmpd was significantly correlated to their water-borne toxicity to rainbow trout.

Bols NC et al; Aquat Toxicol 6 (2): 147-55 (1985)

## Hazardous Substances Data Bank (HSDB)

/AQUATIC SPECIES/ The effective conco of 15 chemicals, inhibiting the cell growth of Scenedesmus subspicatus by 10 and 50% during 96 hr, were investigated in a static test under controlled lab conditions. The most toxic compounds were **pentachlorophenol** and **atrazine**, whereas **benzene**, trichloroethylene, styrene-7,8-oxide, hexachlorobenzene, 1,1-dichloroethylene, and 4-nitrophenol were only slightly toxic. Tris(2,3-dibromopropyl)phosphate, thiourea, 1,2,4-trichlorobenzene, 2,4,6-trichlorophenol, 4-chloroaniline, lindane, and 2,6-dichlorobenzonitrile were of intermediate toxicity. The potential for using this alga as a model test organism is indicated. Gever H et al: Chemosphere 14 (9): 1355-69 (1985)

Hazardous Substances Data Bank (HSDB)

For more Ecotoxicity Excerpts (Complete) data for 1,2,4-TRICHLOROBENZENE (7 total), please visit the HSDB record page

Hazardous Substances Data Bank (HSDB)

## 11.1.19 TSCA Test Submissions

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The ability of 1,2,4-trichlorobenzene (TCB) to induce morphological transformation in the Fischer 344 adult rat liver (ARL) cell line (Cell Transformation Assay) was evaluated in the absence of added metabolic activation. Based on preliminary toxicity tests, TCB was tested using multiple exposures at the highest concentrations that permitted survival (0.001 and 0.005%, v/v) with a time passage following exposure allowing for recovery of the cells. TCB induced a progressive increase in transformation in ARL cells assayed following exposures 5, 9 and 12.

American Health Foundation; Study of the Effects on Cultured Liver Cells of Three Chlorinated Benzenes. (1983), EPA Document No. FYI-AX-0284-0291, Fiche No. 0291-0

Hazardous Substances Data Bank (HSDB)

## 1,2,4-Trichlorobenzene | C6H3Cl3 - PubChem

The ability of 1,2,4-trichlorobenzene (TCB) to cause aberrations in Chinese hamster ovary (CHO) cells in vitro was evaluated in the presence and absence of rat liver S9 metabolic activation. Based on preliminary toxicity tests, nonactivated cultures were treated with 0, 24, 36, 48 or 60 ug TCB/ml (DMSO solvent). None of the test cultures exhibited a significant increase in the frequency of cells with chromosome aberrations in either the activated or nonactivated systems compared to the negative control.

Bioassays Systems Corp.; Effects of 1,2,4-Trichlorobenzene on the In Vitro Induction of Chromosomal Aberrations in Chinese Hamster Ovary Cells. (1982), EPA Document No. 40-8320545, Fiche No. OTS0511274

Hazardous Substances Data Bank (HSDB)

11.1.20 Populations at Special Risk	? Z
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/Individuals who suffer from/ skin, liver, kidney, or chronic respiratory disease, will be at an increased risk if they are exposed to chlorobenzenes. /Chlorobenzenes/

Mackison, F. W., R. S. Stricoff, and L. J. Partridge, Jr. (eds.). NIOSH/OSHA - Occupational Health Guidelines for Chemical Hazards. DHHS(NIOSH) Publication No. 81-123 (3 VOLS). Washington, DC: U.S. Government Printing Office, Jan. 1981., p. 1

## Hazardous Substances Data Bank (HSDB)

#### 11.2 Ecological Information $\bigcirc \ \square$ 11.2.1 US EPA Regional Screening Levels for Chemical Contaminants Resident Soil (mg/kg) 5.80e+00 Industrial Soil (mg/kg) 2.60e+01 Resident Air (ug/m3) 2.10e-01 Industrial Air (ug/m3) 8.80e-01 4.00e-01 Tapwater (ug/L) 7.00e+01 MCL (ug/L) Risk-based SSL (mg/kg) 1.20e-03 MCL-based SSL (mg/kg) 2.00e-01 Oral Slope Factor (mg/kg-2.90e-02 day)-1 Chronic Oral Reference Dose 1.00e-02 (mg/kg-day) **Chronic Inhalation** Reference Concentration 2.00e-03 (mg/m3) Volatile Volatile Fraction of Contaminant Absorbed in Gastrointestinal Tract Soil Saturation 4.04e+02 Concentration (mg/kg)

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

11.2.2 LIS EPA Regional	l Removal Management	Levels for	Chemical Cont	aminants
11.2.2 US LFA Regional	i Kennovai ivianayennent	Levels IOI	Chemical Cont	ammants

Resident Soil (mg/kg)	1.70e+02
Industrial Soil (mg/kg)	7.70e+02
Resident Air (ug/m3)	6.30e+00
Industrial Air (ug/m3)	2.60e+01
Tapwater (ug/L)	1.20e+01
MCL (ug/L)	7.00e+01
Oral Slope Factor (mg/kg- day)-1	2.90e-02
Chronic Oral Reference Dose (mg/kg-day)	1.00e-02
Chronic Inhalation Reference Concentration (mg/m3)	2.00e-03

 $\bigcirc \square$ 

Volatile	Volatile	
Fraction of Contaminant Absorbed in Gastrointestinal Tract	1	
Soil Saturation Concentration (mg/kg)	4.04e+02	
US EPA Regional Screening Levels for Chemical Contaminants at Superfund Sites		

#### 11.2.3 ICSC Environmental Data

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

ILO International Chemical Safety Cards (ICSC)

## 11.2.4 Environmental Fate/Exposure Summary

1,2,4-Trichlorobenzene's production and use as a solvent in chemical manufacturing, dyes and intermediate, in dielectric fluid, synthetic transformer oils, lubricants and heat-transfer mediums and its use as a coolant in electrical equipment and glass tempering may result in its release to the environment through various waste streams; it's former use as an insecticide may have resulted in its direct release to the environment. If released to air, a vapor pressure of 0.46 mm Hg at 25deg C indicates 1,2,4-trichlorobenzene will exist solely as a vapor in the atmosphere. Vapor-phase 1,2,4-trichlorobenzene 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 30 days. The half-life of 1,2,4-trichlorobenzene in surface waters, when exposed to summer sunlight at 40 deg latitude, was calculated as 450 years, suggesting that the compound is not expected to be susceptible to direct photolysis by sunlight. If released to soil, 1,2,4-trichlorobenzene is expected to have moderate to no mobility based upon Koc values of 440 to 10,715. Volatilization from moist soil surfaces is expected to be an important fate process based upon a Henry's Law constant of 1.42X10-3 atm-cu m/mole. However, adsorption to soil is expected to attenuate volatilization. 1,2,4-trichlorobenzene is expected to adsorb to suspended solids and sediment based upon the Koc values. The aerobic and anaerobic biodegrade slowly in soils, with biodegrade slowly and solid as ester was reported as 28 and 110 days, respectively. Volatilization from water sunfaces is expected to be attenuated volatilization from water suffaces is expected to be deaded by a sorption is considered. Measured BCF values of 120 in carp to 57,544 in Atlantic croaker suggest bioconcentration in aquatic organism is high to very high. A nydrolysis half-life was given as 3.4 years for 1,2,4-trichlorobenzene via inhalation of food and drinking water, and dermal contact with this compound at wor

Hazardous Substances Data Bank (HSDB)

#### 11.2.5 Artificial Pollution Sources

1,2,4-Trichlorobenzene's production and use as a solvent in chemical manufacturing, dyes and intermediate, in dielectric fluid, synthetic transformer oils, lubricants and heat-transfer mediums(1) and its use as a coolant in electrical equipment and glass tempering(2) may result in its release to the environment through various waste streams; its former use as an insecticide(1) may have resulted in its direct release to the environment(SRC).

(1) Lewis RJ; Hawley's Condensed Chemical Dictionary. 15th ed. NY,NY: Van Nostrand Reinhold Co., p. 1265 (2007) (2) Rogers HR; Sci Total Environ 185: 3-26 (1996)

## Hazardous Substances Data Bank (HSDB)

## 11.2.6 Environmental Fate

TERRESTRIAL FATE: Based on a classification scheme(1), Koc values of 440(2) to 10,715(3), indicate that 1,2,4-trichlorobenzene is expected to have moderate to no mobility in soil(SRC). Volatilization of 1,2,4-trichlorobenzene from moist soil surfaces is expected to be an important fate process(SRC) given a Henry's Law constant of 1.42X10-3 atm-cu m/mole(4). However, adsorption to soil is expected to attenuate volatilization(SRC). 1,2,4-Trichlorobenzene is not expected to volatilize from dry soil surfaces(SRC) based upon a vapor pressure of 0.46 mm Hg(5). 1,2,4-Trichlorobenzene is expected to biodegrade slowly in soils with biodegradation half-lives ranging from several weeks to a few months(6,7).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Rathbun RE; Crit Rev Environ Sci 30:129-295 (2000) (3) Beck AJ et al; Adv Agron 55:345-91 (1995) (4) Warner HP et al; Determination of Henry's Law constants of selected priority pollutants. EPA/600/D-87/229, NTIS PB87-212684 (1987) (5) Shiu WY, Mackay D; J Chem Eng Data 24: 27-30 (1997) (6) Middeldorp PJM et al; Appl Environ Microbiol 63: 1125-9 (1997) (7) Bosma TNP et al; Ground Water 34: 49-56 (1996)

#### Hazardous Substances Data Bank (HSDB)

AQUATIC FATE: Based on a classification scheme(1), Koc values of 440(2) 10,715(3), indicate that 1,2,4-trichlorobenzene is expected to adsorb to suspended solids and sediment(SRC). Volatilization from water surfaces is expected(4) based upon a Henry's Law constant of 1.42X10-3 atm-cu m/mole(5). Using this Henry's Law constant and an estimation method(4), volatilization half-lives for a model river and model lake are 4.8 hours and 5.6 days, respectively(SRC). However, volatilization from water surfaces is expected to be attenuated by adsorption to suspended solids and sediment in the water column. The volatilization half-life from a model pond is up to 86 days when adsorption is considered(6). According to a classification scheme(7), BCF values of 120 in carp(8) to 57,544 in Atlantic croaker(2), suggest bioconcentration in aquatic organisms is high to very high(SRC). A hydrolysis half-life was given as 3.4 years for 1,2,4-trichlorobenzene(2). The aerobic and anaerobic biodegradation half-lives of 1,2,4-trichlorobenzene in natural waters was reported as 28 and 110 days, respectively(9).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Rathburn RE; Crit Rev Environ Sci 30: 129-295 (2000) (3) Back AJ et al; Adv Agron 55: 345-91 (1995) (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9, 15-1 to 15-29 (1990) (5) Warner HP et al; Determination of Henry's Law constants of selected priority pollutants. EPA/600/D-87/229. NIIS P887-212684 (1987) (6) US EPA, EXAMS II Computer Simulation (1987) (7) Franke C et al; Chemosphere 29: 1501-14 (1994) (8) Chemicals Inspection and Testing Institute. Japan Chemical Industry Ecology - Toxicology and Information Center. ISBN 4-89074-101-1 (1992) (9) Capel PD, Larson 5J; Chemosphere 28: 2179-24 (1995)

#### Hazardous Substances Data Bank (HSDB)

AQUATIC FATE: 1,2,4-Trichlorobenzene has estimated half-lives of 0.3-3, 3-30, and 30-300 days in rivers, lakes and groundwater, respectively(1).

(?) [7]

# 0 Z

## 1,2,4-Trichlorobenzene | C6H3Cl3 - PubChem

(1) Zoetman BCJ et al; Natl Inst Water Supply, Presented 3rd Internat Sympo, Aquatic Pollut, Oct 15-17 CBH 79-386 (1979)

## Hazardous Substances Data Bank (HSDB)

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), 1,2,4-trichlorobenzene, which has a vapor pressure of 0.46 mm Hg at 25 °C(2), is expected to exist solely as a vapor in the atmosphere atmosphere. Vapor-phase 1,2,4-trichlorobenzene 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 30 days(SRC), calculated from its rate constant of 5.3X10-13 cu cm/molecule-sec at 25 °C(3). The half-life of 1,2,4-trichlorobenzene in surface waters, when exposed to summer sunlight at 40 deg latitude, was calculated as 450 years(4), suggesting that the compound is not expected to be susceptible to direct photolysis by sunlight(SRC).

(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) Shiu WY, Mackay D; J Chem Eng Data 24: 27-30 (1997) (3) Atkinson R; J Phys Chem Ref Data Monograph No 1 (1989) (4) Dulin D et al; Environ Sci Technol 20: 72-77 (1986)

Hazardous Substances Data Bank (HSDB)

#### 11.2.7 Environmental Biodegradation

2 Z

AEROBIC: A 0% theoretical BOD in sludge over a 2 week incubation period was observed for 1,2,4-trichlorobenzene(1). The aerobic biodegradation half-life of 1,2,4-trichlorobenzene in natural waters has been reported as 28 days(2). An 8-day theoretical BOD of 1% in a **benzene** acclimated sludge was observed for 1,2,4-trichlorobenzene(3). A 20-day theoretical BOD of 0% in municipal wastewater was observed for 1,2,4-trichlorobenzene while 20-day theoretical BODs of 78, 100 and 55% were observed for industrial wastewater(4). 1,2,4-Trichlorobenzene was dechlorinated 0.3-50.1% after 7 days incubation in soil amended with up to 4 mM bromoethanesulfonate, 2 mM **sulfate** and 7.5 mM **hydrogen**(5). After 4 days of incubation 28 uM of 1,2,4-trichlorobenzene was biodegraded to 1,4**dichlorobenzene** and **chlorobenzene**(6). 1,2,4-Trichlorobenzene, under aerobic conditions, degraded 40% in dune sediment taken near Zandvoort, Netherlands after a 2 month lag time(7). 1,2,4-Trichlorobenzene was biodegraded 90% in groundwater samples under aerobic conditions(8). 1,2,4-Trichlorobenzene had influent concns of 90 and 8100 ug/L and effluent concns of <5.0 and <10 ug/L using an activated sludge with a daily mass loading of COD/bacterial mass ratios of 0.3 and 0.6(9).

(1) Chemicals Inspection and Testing Institute. Japan Chemical Industry Ecology - Toxicology and Information Center. ISBN 4-89074-101-1 (1992) (2) Capel PD, Larson SJ; Chemosphere 30: 1097-1106 (1995) (3) Malaney GW, McKinney RE; Water Sew Works 113: 302-309 (1966) (4) Simmons P et al; Text Chem Color 9: 211-13 (1977) (5) Advian L et al; Appl Environ Microbiol 64: 496-503 (1998) (6) Middeldorp PJM et al; Appl Environ Microbiol 63: 1125-9 (1997) (7) Bosma TNP et al; Ground Water 34:49-56 (1996) (8) Davis A, Olsen RL; in Hazardous Materials Control 3, pp 18-37 (1990) (9) Olthof M, Olmstead DG; in Proc Ind Waste Conf. 1992 47th Chelsea, MI pp 83-42 (1993)

#### Hazardous Substances Data Bank (HSDB)

... The formation rate of (14)C labeled carbon dioxide through the biodegradation of 1,2,4-trichlorobenzene (TCB) by activated sludge was examined. After 5 days, 13% of the 1,2,4-trichlorobenzene remained, 56% was converted to carbon dioxide, 23% to polar metabolites, and 7% was volatilized. Approximately 80% of the 1,2,4-trichlorobenzene was adsorbed on solids accounting for the low volatility from the system.

Callahan, M.A., M.W. Slimak, N.W. Gabel, et al. Water-Related Environmental Fate of 129 Priority Pollutants. Volume I. EPA-440/4 79-029a. Washington, DC: U.S. Environmental Protection Agency, December 1979., p. 76-7

#### Hazardous Substances Data Bank (HSDB)

ANAEROBIC: 1,2,4-Trichlorobenzene was biodegraded by an acclimated anaerobic sediment slurry obtained from the Tsurumi River, Japan(1). The first-order biodegradation rate constant was 0.017/days, corresponding to a half-life of about 41 days(1). The half-life of 1,2,4-trichlorobenzene in sewage sludge amended soil was 23 days(2). Sediment from freshwater streams in the Netherlands degraded 1,2,4-trichlorobenzene, with reported biodegradation half-lives of 50-212 days(3). An enriched microbial culture derived from sediment of the Rhine River reductively dechlorinated 1,2,4-trichlorobenzene in about 1 year following a lag period of over 138 days(4). The anaerobic biodegradation half-life of 1,2,4-trichlorobenzene in natural waters has been reported as 110 days(5). Sediment from the Ise Bay, Japan reductively dechlorinated 1,2,4-trichlorobenzene a rate of 15-35 pmols/day, with the main degradation product reported as 1,2-dichlorobenzene(6). 1,2,4-Trichlorobenzene, under methanogenic conditions, degraded 11% in groundwater samples under anaerobic biodegradation rates for 1,2,4-trichlorobenzene was biodegradation rates 0, 0,096/day(9). 1,2,4-Trichlorobenzene was anaerobically biodegraded 50% in <4 days(1).

(1) Masunga S et al; Wat Sci Technol 33: 173-80 (1996) (2) Wang MJ, Jones KC; Environ Sci Technol 28: 1843-52 (1994) (3) Peijnenburg WJGM et al; Environ Toxicol Chem 11: 289-300 (1992) (4) Hollinger C et al; App Environ Microbiol 58: 1636-44 (1992) (5) Capel PD, Larson SJ; Chemosphere 30: 1097-1106 (1995) (6) Yonezawa Y et al; Chemosphere 28: 2179-84 (1994) (7) Bosma TNP et al; Ground Water 34: 49-56 (1996) (8) Davis A, Olsen RL; in Hazardous Materials Control 3, pp 18-37 (1990) (9) Rathbun RE; Crit Rev Environ Sci 30: 129-295 (2000) (10) Rogers HR; Sci Total Environ 185: 3-26 (1996)

#### Hazardous Substances Data Bank (HSDB)

## 11.2.8 Environmental Abiotic Degradation

The rate constant for the vapor-phase reaction of 1,2,4-trichlorobenzene with photochemically-produced hydroxyl radicals is 5.3X10-13 cu cm/molecule-sec at 25 °C(1). This corresponds to an atmospheric half-life of about 30 days at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(1). A hydrolysis half-life was given as 3.4 years for 1,2,4-trichlorobenzene(2). The half-life of 1,2,4-trichlorobenzene in surface waters, when exposed to summer sunlight at 40 deg latitude, was calculated as 450 years(3), suggesting that the compound is not expected to be susceptible to direct photolysis by sunlight(SRC).

(1) Atkinson R; J Phys Chem Ref Data Monograph No 1 (1989) (2) Rathbun RE; Crit Rev Environ Sci 30: 129-295 (2000) (3) Dulin D et al; Environ Sci Technol 20: 72-77 (1986)

Hazardous Substances Data Bank (HSDB)

11.2.9 Environmental Bioconcentration

#### **Bioconcentration Factor**

2.09e+03

EPA DSSTox

BCF values of 420 to 1,140 were measured in carp exposed to 50 ug/L of 1,2,4-trichlorobenzene during a 6 week incubation period and BCF values of 120 to 1,300 were measured in carp exposed to 5 ug/L of 1,2,4-trichlorobenzene during a 6 week incubation period (1). The BCF value of 1,2,4-trichlorobenzene in fish in a flowing water system was 490 while the BCF value for trout in a static water system was 2400(2). Log BCFs of 3.11, 3.51, 3.36 and 3.57 were measured in 4 rainbow trout samples on a whole body basis, and 4.20, 4.57, 4.54 and 4.71 using lipid basis(3). Log BCFs of 3.10, 2.60, 1.91, 3.19, 3.32 and 3.31 were measured in Atlantic croaker, blue crab, spotted sea trout, blue catfish, fathead minnow and flagfish, respectively, on a whole body basis, and at 4.20, 4.57, 4.76, 4.90,

# ⊘ [2

() [7]

## 1,2,4-Trichlorobenzene | C6H3Cl3 - PubChem

3.54, 4.68, 3.45, 4.54, 4.71 and 4.25, respectively, using lipid basis(3). 1,2,4-Trichlorobenzene had a log BCF of 2.95 in guppy (Poecilia reticulata)(4). A BCF of 491 was given for 1,2,4-trichlorobenzene in fish(5). 1,2,4-Trichlorobenzene at concns of 3.2 and 53 ng/L, in a flow-through system showed BCFs of 1300 and 3200, respectively, in rainbow trout exposed over 119 days(6). Fish continuously exposed to a mean measured aqueous concn of 2.9 ug/L of 1,2,4-trichlorobenzene had a estimated equilibrium bioconcentration factor of 182(7). According to a classification scheme(8), these BCF values suggest that bioconcentration in aquatic organisms is high to very high. Daphnids continuously exposed to a mean measured aqueous concn of 3.1 ug/L of 1,2,4-trichlorobenzene had a estimated equilibrium bioconcentration factor of 142(7).

(1) Chemicals Inspection and Testing Institute. Japan Chemical Industry Ecology - Toxicology and Information Center. ISBN 4-89074-101-1 (1992) (2) Prasad SS; J AOAC Int 75: 916-24 (1992) (3) Rathbun RE; Crit Rev Environ Sci 30: 129-295 (2000) (4) Sacan MT et al; J Chem Inf Comput Sci 44: 985-992 (2004) (5) Kenaga EE; Ecotoxocl Environ Safety 4: 26-38 (1980) (6) Oliver BG, Nümi AJ; Environ Sci Technol 17: 287-91 (1983) (7) Callahan MA et al; Water-Related Environmental Fate of 129 Priority Pollutants. V1. EPA-440/4 79-029a. Washington, DC: US Environmental Protection Agency (1979) (8) Franke C et al; Chem osphere 29: 1501-14 (1994)

#### Hazardous Substances Data Bank (HSDB)

#### 1,2,4-Trichlorobenzene BCF values in various fish(1).

Common name	Genus species	BCF wet weight	BCF lipid weight
Rainbow trout	Oncorhynchus mykiss	124; 1,300; 1,600; 1,300; 3,200	6,890; 16,880; 20,780; 15,660; 36,364
Carp	Cyprinus carpio	190; 460; 540	8,636; 10,455; 12,270
Rainbow trout (hatchling)	Oncorhynchus mykiss	349; 710	9,090; 22,188
Golden ide	Leuciscus idus	914	18,280
Zebra fish	Brachidanio rerio	810	15,580
Tilapia	Tilapia nilotica	680; 870	13,080; 16,730
Guppy (female)	Poecilia reticulata	702; 756	13,000; 14,000
Bluegill sunfish	Lepomis macrochirus	960; 1,1320	16,842; 23,160
Guppy	Poecilia reticulata	1,350; 1,380; 910; 1,080	23,280; 23,790; 11,100; 13,170
Fathead minnow	Pimephales promelas	2,100	20,000

(1) Geyer HJ et al; in Handbook Environ Chem. vol. 2, Pt. J, Beek B ed., Springer-Verlag: Berlin, Germany, pp.1-166. (2000)

#### Hazardous Substances Data Bank (HSDB)

Certain developmental stages of Salmo gairdneri accumulated more 1,2,3-trichlorobenzene and 1,2,4-trichlorobenzene ... than others. ... The bioconcentration factor was approximately 10 times as great at hatching as in alevins. These differences can be reduced, but not eliminated, by expressing the data on the basis of lipid wt.

Galassi S, Calamari D; Chemosphere 12 (11-12): 1599-603 (1983)

#### Hazardous Substances Data Bank (HSDB)

Contaminated food was prepared by exposing pink shrimp (Penaeus duorarum) to 10 ug/L 1,2,4-trichlorobenzene -UL-(14)C for 12 days; whole body concn of trichlorobenzene in the exposed shrimp was 0.59 ug/g. Juvenile spot (Leiostomus xanthurus) were fed the trichlorobenzene contaminated shrimp at a daily ration of 10% body wt for 28 days; they accumulated <0.05 ug/g trichlorobenzene (detection limits). Spot, exposed to 10 ug/L trichlorobenzene in water for 28 days and fed uncontaminated food, bioconcentrated trichlorobenzene approximately 100 times the aqueous exposure conc. Spot, exposed simultaneously to contaminated food and water described above, bioaccumulated trichlorobenzene equal to the aqueous exposure treatment. Results were compared with data from a trichlorobenzene bioaccumulation with freshwater species; both studies indicated that trichlorobenzene was accumulated moderately from contaminated food was negligible.

Heitmuller PT, Clark JR; Govt Reports Announcements & Index (GRA&I), Issue 06, 1990

#### Hazardous Substances Data Bank (HSDB)

11.2.10 Soil Adsorption/Mobility	2 (2)

## Soil Adsorption Coefficient

## 1.26e+03 L/kg

EPA DSSTox

Measured log Kocs of 3.1(1), 3.30(2), 3.35(3), 3.96(4-5), 4.03(6) were reported for 1,2,4-trichlorobenzene in soil. Koc values for 1,2,4-trichlorobenzene were 864 and 440 in soil and peaty soil(7). Log Koc values for peat soil and Dover soil taken from Zhejiang Province, China were 3.06 and 3.58(8). According to a recommended classification scheme(9), these Koc values suggest that 1,2,4-trichlorobenzene has moderate to no mobility in soil.

(1) Sacan MT, Balcioglu IA; Chemosphere 32: 1993-2001 (1996) (2) Xu F et al; J Environ Qual 30: 1618-23 (2001) (3) Borisover MD, Graber ER; Chemosphere 34: 1761-76 (1997) (4) Chu W, Chan K-H; Sci Total Environ 248: 1-10 (2000) (5) Gao C et al; Environ Toxicol Chem 15: 1089-96 (1996) (6) Beck AJ et al; Adv Agron 55: 345-91 (1995) (7) Rathbun RE; Crit Rev Environ Sci 30: 129-295 (2000) (8) Yang K et al; Chemosphere 61: 116-28 (2005) (9) Swann RL et al; Res Rev 85: 23 (1983)

#### Hazardous Substances Data Bank (HSDB)

A log Koc value of 3.9 was measured for 1,2,4-trichlorobenzene in sediment obtained from Ise Bay, Japan(1). A log Koc value of 5.0 was measured from sediment of Lake Ketelmeer, Netherlands(2). Log Koc values of 6.12 and 5.50 were also measured in Lake Ketelmeer at 0-30 cm (3.75% organic matter) and 40-120 cm (6.48% organic matter), respectively(3). The log Koc was reported as 4.06 in landfill effluent(4). 1,2,4-Trichlorobenzene had reported log Kocs of 4.56 and 4.74 in sediments from Bayou d'Inde and Calcosieu River, on Lake Charles, LA(5). A log Koc of 3.42 was reported in Dickenson sediment(6). A log Koc of 5.62 was found in sediment for 1,2,4-trichlorobenzene(7). Log Kocs of 3.30-4.18, 3.6, and 3.93 were reported in estuarine sediment(8). Koc values of 2350 and 3250 were given for aquifer material and sediment for 1,2,4-trichlorobenzene(9).

## 1,2,4-Trichlorobenzene | C6H3Cl3 - PubChem

(1) Masunga S et al; J Environ Sci Health A31: 887-903 (1996) (2) ten Hulscher TEM et al; Chemosphere 35: 2331-44 (1997) (3) Jonker MTO, Smedes F; Environ Sci Technol 34: 1620-6 (2000) (4) Brack W et al; Environ Toxicol Chem 17:1982-91 (1998) (5) Chen W et al; Environ Toxicol Chem 18: 1610-6 (1999) (6) Chen W et al; Environ Sci Technol 34: 385-92 (2000) (7) Ditoro DM, McGrath JA; Environ Toxicol Chem 19: 1971-82 (2000) (8) Gess P, Pavlostathis SG; Environ Toxicol Chem 16: 1598-1605 (1997) (9) Rathbun RE; Crit Rev Environ Sci 30: 129-295 (2000)

#### Hazardous Substances Data Bank (HSDB)

## 1,2,4-Trichlorobenzene Koc values at differing soil depth in Duke Forest soils(1)...

Soil Horizon (depth, cm)	Кос	Soil Depth cm	pH; % TOC; % Sand; % Silt; % Clay
A (0-28)	2,850	0-28	3.9; 0.536; 91.0; 8.4; 0.6
E (28-41)	2,200	28-41	4.6; 0.191; 74.7; 13.9; 11.4
EB (41-61)	1,500	41-61	4.4; 0.098; 67.7; 16.9; 15.4
BE (61-84)	1,200	61-84	4.4; 0.127; 0.127; 41.9; 17.3; 40.8
B1 (84-134)	640	84-134	5.2; 0.099; 23.4; 20.4; 56.2
B2 (134-184)	500	134-184	4.4; 0.079; 0.079; 25.4; 23.2; 51.4
B3 (184-234)	290	184-234	4.6; 0.063; 27.2; 26.0; 46.8

(1) Kimaninjoroge BN et al; J Contam Hydrol 29: 347-77 (1998)

#### Hazardous Substances Data Bank (HSDB)

## 11.2.11 Volatilization from Water/Soil

The Henry's Law constant for 1,2,4-trichlorobenzene is 1.42X10-3 atm-cu m/mole(1). This Henry's Law constant indicates that 1,2,4-trichlorobenzene is expected to volatilize from water surfaces(2). Based on this Henry's Law constant, the volatilization half-life from a model river (1 m deep, flowing 1 m/sec, wind velocity of 3 m/sec)(2) is estimated as 4.8 hours(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 5.6 days(SRC). However, 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 5.6 days(SRC). However, volatilization half-life from a model pond is up to 86 days when adsorption to suspended solids and sediment in the water column. The volatilization half-life from a model pond is up to 86 days when adsorption is considered(3). 1,2,4-Trichlorobenzene's Henry's Law constant indicates that volatilization from moist soil surfaces may occur(SRC). 1,2,4-Trichlorobenzene is not expected to volatilize from dry soil surfaces(SRC) based upon a vapor pressure of 0.46 mm Hq(4).

(1) Warner HP et al; Determination of Henry's Law constants of selected priority pollutants. EPA/600/D-87/229, NTIS PB87-212684 (1987) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990) (3) US EPA; EXAMS II Computer Simulation (1987) (4) Shiu WY, Mackay D; J Chem Eng Data 24: 27-30 (1997)

### Hazardous Substances Data Bank (HSDB)

## 11.2.12 Environmental Water Concentrations

DRINKING WATER: Drinking water samples from three cities in the Lake Ontario vicinity contained 1,2,4-trichlorobenzene at a mean concn of 2 parts per trillion(1). 1,2,4-Trichlorobenzene was detected in bank filtered Rhine River tapwater at concns of greater than 5 ppb(2). 1,2,4-Trichlorobenzene was detected in 100 of 110 drinking water samples collected in 11 US cities at an avg concn of 0.09 ppb(3). 1,2,4-Trichlorobenzene was identified, not quantified, in drinking water from Milan, Italy(4).

(1) Oliver BG, Nicol KD; Environ Sci Tech 16: 532-6 (1982) (2) Piet GJ et al; pp. 69-80 In Hydrocarbon Halo Hydrocarbon Aquatic Environ Afghan BK, Mackay D Ed. (1980) (3) McNamara PW et al; Exposure And Risk Assessment For 1,2,4-Trichlorobenzene. USEPA-440/4-85-017 (1981) (4) Botta D et al; Environ Sci Technol 30: 453-62 (1996)

#### Hazardous Substances Data Bank (HSDB)

GROUNDWATER: 1,2,4-Trichlorobenzene was found in groundwater pumping stations in the Netherlands at a max concn of 1.2 ppb(1). 1,2,4-Trichlorobenzene was not detected (detection limit 0.188 ug/L) in 78 wells (15 agricultural, 30 new urban, 20 old urban, 13 undeveloped) in Glassboro, NJ(2). 1,2,4-Trichlorobenzene was detected in ground water at Toms River superfund site, NJ at concns of 4.43-5.02 mg/L(3). 1,2,4-Trichlorobenzene was detected in 2% of 214 ground water samples from 30 industrial areas in Taiwan(4). 1,2,4-Trichlorobenzene was identified, not quantified, downstream from 92 waste disposal sites(5). 1,2,4-Trichlorobenzene had an avg ground water concn of 0.002 ug/L in localities contaminated by agrochemical and communal waste in Slovakia(6). A maximum 1,2,4-trichlorobenzene concn of 1.2 ug/L was found in groundwaters in The Netherlands(7).

(1) Zoeteman BCJ et al; Chemosphere 9: 231-49 (1980) (2) Baehr AL et al; Water Resour Res 35: 127-36 (1999) (3) Carmichael LM et al; J Environ Qual 28: 888-97 (1999) (4) Kuo MCT et al; Bull Environ Contam Toxicol 65: 654-9 (2000) (5) Oman C; Int J Environ Anal Chem 71: 73-85 (1998) (6) Veningerova M et al; J Chromatogr A 774: 333-47 (1997) (7) Zoeteman BCJ et al; Chemosphere 9: 231-49 (1980)

#### Hazardous Substances Data Bank (HSDB)

SURFACE WATER: 1,2,4-Trichlorobenzene was detected at a mean concn of 11 parts per trillion in the Niagara River(1). 1,2,4-Trichlorobenzene was detected at mean concns of 0.10 ng/L (Edwards Point) and 0.09 ng/L (Port Lambton) in Ontario, Canada(2). 1,2,4-Trichlorobenzene was detected at mean concns of 0.54, 0.19 and 0.29 ng/L in Lake Ontario(3). 1,2,4-Trichlorobenzene was detected in 100% of samples taken at 21 stations on Lake Erie in 1986 at concns of 0.281-0.714 ng/L(4).

(1) Oliver BG; Symp Am Chem Soc, Div Environ Chem 186th Natl mtg 23: 421-2 (1983) (2) Chan CH; Wat Pollut Res J Canada 28: 451-71 (1993) (3) Halfon E, Poulton D; Water Poll Res J Canada 27: 751-72 (1992) (4) Wang J, Xie Y; Environ Technol 15: 701-14 (1994)

#### Hazardous Substances Data Bank (HSDB)

SURFACE WATER: 1,2,4-Trichlorobenzene was detected at concns of 0.03-0.11 ug/L in Lake Ketelmeer, Netherlands(1). 1,2,4-Trichlorobenzene was detected in rivers in Osaka, Japan at a mean concn of 0.16 ug/L(2). 1,2,4-Trichlorobenzene was detected at median concns of 45, 90 and 80 ng per cubic decimeter in the Scheldt estuary, Netherlands(3). 1,2,4-Trichlorobenzene was detected at mean concns of 8,100 ng/L (Besos River), 1,200 ng/L (Llobregat River), 5.4 ng/L (coastal waters), 8.1 ng/L (Barcelona coastal waters) and 3.6 ng/L (La Pineda coastal waters) in Spain(4). 1,2,4-Trichlorobenzene was detected at concns of 0.1-29.1 ng/L in Ise Bay, Japan(5). 1,2,4-Trichlorobenzene was detected at the survey stations of Zollenspieker at 3-24 ng/L in 12 of 20 samples and Seemannshoft at 3.0-22 ng/L in all 20 samples, on the River Elbe, near Hamburg, Germany in 1992(6). 1,2,4-Trichlorobenzene was detected at 0.019, 0.003 and 0.010 ug/L in Huanchao River, Tanking River near a factory, and the middle of Tanking River in Jiangsu Province, China, respectively(7). 1,2,4-Trichlorobenzene was detected at approximately 10, 7, 1,5, and 1.5% of the total chlorobenzenes found in samples from Aire, Calder, Don, and Trent Rivers, Humber, respectively; samples were taken Feb 1995 to Feb 1997(9). Dutch surface water samples taken from 1992 to 1997 from the Rhine, Meuse and northern delta area, were

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## 1,2,4-Trichlorobenzene | C6H3Cl3 - PubChem

reported as <0.1 ug/L, and Westerscheld was reported as 0.2 ug/L of 1,2,4-trichlorobenzene(10). 1,2,4-Trichlorobenzene had an avg surface water concn of 0.005 ug/L in localities contaminated by agrochemical and communal waste in Slovakia(11). 1,2,4-Trichlorobenzene was detected in 3 of 106 urban shallow rivers in Osaka, Japan in samples taken 1995 to 1997(12). A 1,2,4-trichlorobenzene concn of 1 ug/L was found in the Rhine River at Lobith, Netherlands in July 1979(13).

(1) ten Hulscher TEM et al; Chemosphere 35: 2331-44 (1997) (2) Yamamoto K et al; Environ Pollut 95: 135-43 (1997) (3) van Zoest R, van Eck GTM; Sci Total Environ 103: 57-71 (1991) (4) Gomez-Belinchonen JI et al; Water Res 25: 577-89 (1991) (5) Masunga S et al; Wat Res 25: 289-97 (1991) (6) Gotz R et al; Chemosphere 36: 2085-101 (1998) (7) Huang Z et al; Bull Environ Toxicol T1: 1026-33 (2003) (8) Martinez E et al; J Environ Monit 4: 253-7 (2002) (9) Meharg AA et al; Sci Total environ 251/252: 243-53 (2000) (10) Miermans CJH et al; Chemosphere 40: 39-48 (2000) (11) Veningerova M et al; J Environ Monit 4: 253-7 (2002) (9) Meharg AA et al; Sci Total environ 251/252: 243-53 (2000) (10) Miermans CJH et al; Chemosphere 40: 39-48 (2000) (11) Veningerova M et al; J Environ Monit 4: 253-7 (2002) (9) Meharg AA et al; Sci Total environ 251/252: 243-53 (2000) (10) Miermans CJH et al; Colora (2001) (13) Zoeteman BC et al; Chemosphere 9: 231-49 (1980)

#### Hazardous Substances Data Bank (HSDB)

RAIN/SNOW: 1,2,4-Trichlorobenzene was detected in 1 of 4 rain events in central Portland, OR at a concn of 0.1 parts per trillion and in 2 of 5 rain events in southern Portland at 0.086 and 0.11 parts per trillion(1). 1,2,4-Trichlorobenzene was detected in 3 of 7 rainfall events at an avg concn of 0.25 parts per trillion, collected in Portland, OR from February-April 1984(2). 1,2,4-Trichlorobenzene was identified at 1 of 10 snow sample sites in Russia and Finland; 2.60 ug/kg at Moscow State University (Moscow, Russia)(3).

(1) Pankow JF et al; Environ Sci Technol 18: 310-18 (1984) (2) Ligocki MP et al; Atmos Environ 19: 1609-17 (1985) (3) Poliakova OV et al; Toxicol Environ Chem 75: 181-94 (2000)

## Hazardous Substances Data Bank (HSDB)

## 11.2.13 Effluent Concentrations

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1,2,4-Trichlorobenzene was detected in the ash of municipal waste incinerators in the US at concns of 250 and 81 ug/kg(1). 1,2,4-Trichlorobenzene was detected at a concn of 0.55 ug/cu m in the effluent of a hazardous waste incinerator in Germany(2). 1,2,4-Trichlorobenzene was detected at mean concns of <0.05 to 0.07 mg/cu m in the air of municipal landfills in Finland(3). The emission rate of 1,2,4-trichlorobenzene in the US is 186 tons/yr(4). 1,2,4-Trichlorobenzene was detected in the effluent of New York City municipal wastewater at a concn of 30 ug/L(5) and in the effluent of pulp mills in Finland at concns of 0.7 and 2.8 ug/L(6). 1,2,4-Trichlorobenzene was detected at an avg conc of 2.63 mg/kg in sewage sludge from the UK(7). 1,2,4-Trichlorobenzene was not detected (detection limit 1 ug/L) in leachate from six asphalt pavement reclamation locations in FL(8). 1,2,4-Trichlorobenzene was detected at 0.02-4.8 mg/kg in sewage sludge in the UK(9). 1,2,4-Trichlorobenzene was encours of 0.0015, 0.01, 0.10 and 0.01 ug/L and in solids from runoff, primary sludge and treated sludge at 8.5, 9.3 and 14.8 ug/kg, respectively, in areas of concern in Ontario(10). 1,2,4-Trichlorobenzene had an avg concn of 0.28 ug/L with a frequency of 1.4% in trade effluents(11). Effluent from a municipal waste pilot combustion facility had an avg emission of 537.0 ng/cu m of 1,2,4trichlorobenzene (12). 1,2,4-Trichlorobenzene was detected in leachates from 3 waste disposal sites at concns of 9 and 10, 490, and 4000 ug/L(13). The max observed concn of 1,2,4-trichlorobenzene in air from 8 solid waste composting facilities in the US was 9 ug/cu m(14).

(1) Shane BS et al; Arch Environ Contam Toxical 19: 665-73 (1990) (2) Jay K, Stieglitz L; Chemosphere 30: 1249-60 (1995) (3) Assmuth T, Kalevi K; Chemosphere 24: 1207-16 (1992) (4) Dempsey CR J Air Waste Manage Assoc 43: 1374-79 (1993) (5) Stubin AI et al; Wat Environ Res 68: 1037-44 (1996) (6) Juutti S et al; Chemosphere 32: 1373-40 (1996) (7) Beck AI et al; Adv Agron 55: 345-91 (1995) (8) Brantley AS, Tovarsend TG; Environ Eng Sci 16:105-16 (1999) (9) Rogers HR; Sci Total Environ 185: 3-26 (1996) (10) Schroeter HO; Water Qual Res J Can 32: 7-22 (1997) (11) Stangroom SJ et al; Environ Technol 19: 643-66 (1998) (12) Zimmermann R et al; Environ Sci Technol 35: 1019-30 (2001) (13) Brack W et al; Environ Toxicol Chem 17: 1982-91 (1998) (14) Eitzer BD; Environ Sci Technol 29: 886-902 (1995)

#### Hazardous Substances Data Bank (HSDB)

1,2,4-Trichlorobenzene was detected in municipal waste water at Port Loma sewage treatment plant, at concn of 0.23 ug/L (Fall, 1976) and 0.01 ug/L (Summer, 1976). 1,2,4-Trichlorobenzene was detected in municipal waste water at Oxnard, CA sewage treatment plant at concn of 0.9 ug/L (Fall) and 0.25 ug/L (Summer). 1,2,4-Trichlorobenzene was detected in municipal waste water at the Orange County Sewage Dept, LA at a concn of 0.30 ug/L. 1,2,4-Trichlorobenzene was detected in 5 mile effluent and municipal waste water at the sewage treatment works, Hyperion, LA, at concn of 6.7 and 3.1 ug/L, respectively. 1,2,4-Trichlorobenzene was detected in municipal waste water at the Joint Water Pollution Control Plant (location not specified), at concn of 6.0 ug/L (Fall) and 1.8 ug/L (Summer, 1976). 1,2,4-Trichlorobenzene was detected in industrial discharge at Chattanooga Creek, TN, at a concn of 500 ug/L (Spring, 1976).

USEPA; Ambient Water Quality Criteria Doc: Chlorinated Benzenes p.C-30 (1980) EPA 440/5-80-028

#### Hazardous Substances Data Bank (HSDB)

#### 11.2.14 Sediment/Soil Concentrations

SEDIMENTS: Lake Ontario, Niagara River area, 6 sites, 20 m sediment traps, 1982, 22-55 ppb; 3 stations, sediment traps at 4 depths 20-68 m deep, avgs 34-41 ppb(2). 1,2,4-Trichlorobenzene was detected in one of 3 sediment samples from Lake Pontchartrain, LA at 3.4 ppb dry weight, date not given(1). West Germany, 7 lakes, 29% pos, detected, not quantified(3). US STORET database, 353 samples, 0.6% pos, median <500 ppm(4). Concn (ppm dry wt) in seds: Southern Lake Huron, 9 samples, 1.5-6.6, 4.3 avg; Lake St. Clair, 2 samples, 1.7-2.5, 2.1 avg; Western Lake Erie, 9 samples, 1.3-14, 5.3 avg; Central Lake Erie, 22 samples, 1.2-3.4, 2.3 avg; Eastern Lake Erie, 15 samples, 1.3-3.5, 2.4 avg(5). 1,2,4-Trichlorobenzene was found in 0.2% of 517 sites sampled from 19 major river basins from Aug 1992 to Sept 1995 with a maximum concn of 68 ug/kg dry weight(6). 1,2,4-Trichlorobenzene was detected in the Calcasieu River estuary, LA at 0-26 mg/kg(7).

(1) McFall JA et al; Chemosphere 14: 1561-9 (1985) (2) Kuntz KW; Toxic Contam in the Niagara River 1975-82 Burlington, Ontario Tech Bull No.134 (1984) (3) Buchert H et al; Chemosphere 10: 945-56 (1981) (4) Staples CA et al; Environ Toxicol Chem 4: 131-42 (1985) (5) Oliver BG, Bourbonniere RA; J Great Lakes Res 11: 366-72 (1985) (6) Lopes TJ, Furlong ET; Environ Sci Technol 20: 727-37 (2001) (7) Bedmond MS et al; Arch Environ Contam Toxicol 30: 53-61 (1996)

#### Hazardous Substances Data Bank (HSDB)

SEDIMENT: 1,2,4-Trichlorobenzene was detected in the sediment of Lake Ketelmeer, Netherlands at concns of 240 and 70(1), 250-400(2) and 24 ug/kg (dry weight)(3), 1,2,4-Trichlorobenzene was detected in sediment of Lake Ladoga, Russia at concns of 2.3-6.8 pg/g(4). 1,2,4-Trichlorobenzene was detected at concns of 1.6-25.3 ng/g in sediment from Ise Bay, Japan(5). 1,2,4-Trichlorobenzene was identified, not quantified, in the sediment of 7 rivers and ports in Niigata, Japan(6). 1,2,4-Trichlorobenzene was detected at median concns of 87, 45, 27 and 14 ng/g in sediment taken from the Scheldt estuary, Netherlands(7). 1,2,4-Trichlorobenzene was detected in sediment off the coast of Taiwan at concns of 1.12 ng/kg(8). 1,2,4-Trichlorobenzene was detected at Median concns of 2002 at the concn of 0.19, not detected, and 0.39-0.63 mg/kg at Xiao Zui, Huaihe River bridge, and Hongguang Chemical plant, respectively(9). 1,2,4-Trichlorobenzene was not detected (detection limit 2 ng/g) in seven river mouths (Tainai, Agano, Shinano, Sekiya, Hokura, Seki, and Oumli rivers) and a port (Prefecture) in Niigata, Japan(10). 1,2,4-Trichlorobenzene was detected at Saone, Chasse, Beauchastel, Donzere and Arles at 6.8, 22.0, 76.7, 27.7 and 67.6 ug/kg (dry weight), respectively(12). Bed sediment samples taken from the Rhone River had concns of 1,2,4-Trichlorobenzene was detected in sediment in 7 of 7 sites in the German Bight area(13).

(1) Beurskens JEM et al; Water Sci Technol 29: 77-85 (1994) (2) ten Hulscher TEM et al; Chemosphere 35: 2331-44 (1997) (3) ten Hulscher TEM et al; Environ Toxicol Chem 23: 1634-9 (2004) (4) Ristola T et al; Chemosphere 32: 1179-92 (1996) (5) Masunga S et al; Wat Res 25: 289-97 (1991) (6) Kawata K et al; Bull Environ Toxicol Chem 23: 1634-9 (2004) (4) Ristola T et al; Chemosphere 32: 1179-92 (1996) (5) Masunga S et al; Wat Res 25: 289-97 (1991) (6) Kawata K et al; Bull Environ Contam Toxicol 58: 893-900 (1997) (7) van Zoest R, van Eck GTM; Sci Total Environ 103: 57-71 (1991) (8) Lee CL, Fang MD; Chemosphere 35: 2039-50 (1997) (9) Huang H et al; Bull Environ Contam Toxicol 73: 339-46 (2004) (10) Kawata K et al; Bull Environ Contam Toxicol 58: 893-900 (1997) (11) Lee CL et al; Chemosphere 35: 2039-50 (1997) (9) Huang H et al; Bull Environ Contam Toxicol 73: 339-46 (2004) (10) Kawata K et al; Bull Environ Contam Toxicol 56: 291-42 (1994) (13) Schwarzbauer J et al; Cog Geochem 31: 11713-31 (2000)

Hazardous Substances Data Bank (HSDB)

SOIL: 1,2,4-Trichlorobenzene was detected in soil at Toms River superfund site, NJ at concns of not detected to 440 ug/kg(1). 1,2,4-Trichlorobenzene was not detected in 705 soil samples taken from 30 industrial areas in Taiwan(2). 1,2,4-Trichlorobenzene had an avg soil concn of 0.021 mg/kg in localities contaminated by agrochemical and communal waste in Slovakia(3).

(1) Carmichael LM et al; J Environ Qual 28: 888-97 (1999) (2) Kuo MCT et al; Bull Environ Contam Toxicol 65: 654-9 (2000) (3) Veningerova M et al; J Chromatogr A 774: 333-47 (1997)

#### Hazardous Substances Data Bank (HSDB)

## 11.2.15 Atmospheric Concentrations

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In a study of aerial fallout in southern California (Spring 1976), five sampling sites showed median 1,2,4-trichlorobenzene levels of less than 11 ng/sq m/day.

USEPA; Ambient Water Quality Criteria Doc: Chlorinated Benzenes p.C-35 (1980) EPA 440/5-80-028

## Hazardous Substances Data Bank (HSDB)

URBAN/SUBURBAN: In 1981, 1,2,4-trichlorobenzene was detected in the air of Oakland and Los Angeles, CA at mean concns of 3 and 7 parts per trillion, respectively; mean concns of trichlorobenzene from Riverside and Torrence, CA, assumed to be of the 1,2,4isomer, were 10 and 360 parts per trillion, respectively(1). The avg concn of 1,2,4-trichlorobenzene in Portland, OR was reported as 3.8 ng/cu m(2). In 1979, mean (range) concns of 1,2,4-trichlorobenzene detected in air from Los Angeles, Phoenix, AZ and Oakland, CA were 69.3 (19.7-339.4), 30.8 (8.7-101.5) and 29.5 (9.7-151.2) parts per trillion, respectively(3). 1,2,4-Trichlorobenzene was detected in 1 US urban location at concns of 0-315 ug/cu m with a mean concn of 3.71 ug/cu m, and in Lima, OH at concns of <0.56 ug/cu m(4). The median concn of 1,2,4-trichlorobenzene in homes in Finland was reported as 0.10 ug/cu m(5). Samples taken Mar 20, 1996 to April 16, 1997 from Porto Alegre, Brazil had 1,2,4-trichlorobenzene concns of not detected to 0.1 ppb(6). 1,2,4-Trichlorobenzene was detected at 2.8, 2.9 and 0.41 ng/cu m in samples taken from Georgetown, North Inlet, SC and Green Bay, WI, respectively(8).

(1) Grosjean D; Sci Total Environ 100: 367-414 (1991) (2) Ligocki MP et al; Atmos Environ 19: 1609-17 (1985) (3) Singh HB et al; Atmos Measurements of Selected Toxic Organic Chem NTIS PB80-19889 (1980) (4) Kelly TJ et al; Ambient Concentration Summaries For Clean Air Act Title III Hazardous Air Pollutants USEPA/600/R-94/090 (1993) (5) Kostiainen R; Atmos Environ 6: 693-702 (1995) (6) Grosjean E et al; Environ Sci Technol 33: 1970-8 (1999) (7) Islam MA, Stancheva E; Water Air Soil Pollut 115: 309-20 (1999) (8) McConnell LL, Bidleman TF; Chemosphere 37: 885-98 (1998)

#### Hazardous Substances Data Bank (HSDB)

#### SOURCE DOMINATED: 1,2,4-Trichlorobenzene was detected in waste dump atmospheric samples at 1474 and 442 ng/cu m in Sabinanigo, Spain(1).

(1) Nerin C et al; Int J Environ Anal Chem 65: 83-94 (1996)

## Hazardous Substances Data Bank (HSDB)

RURAL/REMOTE: 1,2,4-Trichlorobenzene was identified, not quantified, over the western Pacific between Japan and Singapore in Sept 1994(1).

(1) Quack B, Suess E; J Geophys Res 104: 1663-78 (1999)

## Hazardous Substances Data Bank (HSDB)

INDOOR: Indoor data collected from buildings in the Netherlands, Germany, Italy, and USA show 1,2,4-trichlorobenzene levels of <1 ug/cu m in dwellings(1). 1,2,4-Trichlorobenzene was found at a mean concn of 12.8 ug/cu m in 35 homes in WV(2). In samples taken in 754 residences in Canada in 1991 concns of 1,2,4-trichlorobenzene were not detected in samples taken winter and fall and 0.03 ug/cu m in samples taken in spring and summer(3). 1,2,4-Trichlorobenzene was found at detectable levels in 2 of 757 Canadian residences in samples taken in 1992(4). The mean concn of 1,2,4-trichlorobenzene measured in houses in Kuwait from Dec 1994 to Jan 1995 was 284 ug/cu m(5).

(1) Brown SK et al; Indoor Air 4: 123-34 (1994) (2) Crump D; in Organic Indoor Air Pollutants. Occurrence, Measurement, Evaluation. Salthammer T ed, Wiley-VCH: NY, NY pp 57-71 (1999) (3) Fellin P, Otson R; Atmos Environ 28: 3581-6 (1994) (4) Otson R; ASTM Spec Tech Publ 1261: 66-76 (1996) (5) Bouhamra WS et al; Environ Intl 23: 197-204 (1997)

Hazardous Substances Data Bank (HSDB)

#### 11.2.16 Food Survey Values

1,2,4-Trichlorobenzene was detected in corn oil at 0.01 ppm and sunflower oil at 0.003 ppm(1). 1,2,4-Trichlorobenzene was identified, not quantified, in rape seed, walnuts and poppies, soybeans, sesame, and hazelnut(1). 1,2,4-Trichlorobenzene was detected in potatoes at 0.032 ug/kg (peel), cabbage at 0.0159 ug/kg (outer), cauliflower at 0.0104 ug/kg (stem), lettuce at 0.007 ug/kg (outer), and peas at 0.0159 (pod) and 0.0676 ug/kg (seeds)(2). (1) Peattie ME et al; Sci Total Environ 34: 73-86 (1984) (2) Wang MJ, Jones KC; J Agric Food Chem 42: 2322-28 (1994)

Hazardous Substances Data Bank (HSDB)

#### 11.2.17 Plant Concentrations

1,2,4-Trichlorobenzene was identified, not quantified, in plant material grown in an Illinois coal refuse reclamation site(1). 1,2,4-Trichlorobenzene was present in plants at an avg concentration of 0.002 mg/kg in localities contaminated by agrochemical and communal waste in Slovakia(2).

(1) Webber MD et al; J Environ Qual 23: 1019-26 (1994) (2) Veningerova M et al; J Chromatogr A 774: 333-47 (1997)

Hazardous Substances Data Bank (HSDB)

## 11.2.18 Fish/Seafood Concentrations

1,2,4-Trichlorobenzene was detected in trout from the Great Lakes at concns of 0.5-5 ppb(1) and detected in flatfish off the coast of California at concns of <3.4 ppb to 26 ppb(2). 1,2,4-Trichlorobenzene was found in various species of fish from Rivers in Slovenia and from the Gulf of Triest, Yugoslavia 1978, in concns of 1-15 ng/g (dry weight)(3). 1,2,4-Trichlorobenzene was detected in 53% of fish at the 400 sites sampled in the US at a mean concn of 3.1 ng/g(4). 1,2,4-Trichlorobenzene was detected at mean concns of 4.77 ug/g in

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carp, 0.30 ug/kg in white sucker, 0.37 ug/kg in catfish, 0.19 ug/kg in largemouth bass, 0.59 ug/kg in smallmouth bass and 0.38 ug/kg in walleye pike(4). 1,2,4-Trichlorobenzene was detected at 21.19-35.34 ug/g in mussels (Elliptio complanata) from the Cornwall/Massena area on the St Lawrence River in samples taken Sept 28, 1989(5). 1,2,4-Trichlorobenzene was detected in zebra mussel (Dreissena polymorphia) at 1.6 and 1.8 ug/kg (wet weight) sampled at Lobith on the Rhine and Eijsden on the Meuse(6). 1,2,4-Trichlorobenzene was detected at 1.1-330 ng/g (wet weight) in snow crab (Chionoectes opilio) at 13 locations, in samples taken 1996 to 2000(7).

(1) Oliver BG, Nicol KD; Environ Sci Tech 16: 532-6 (1982) (2) Young DR et al; Wat Chlorination Environ Impact Health Effects 3: 471-86 (1980) (3) Jan J, Malnersic S; Bull Environ Contam Toxicol 24: 824-7 (1980) (4) Kuehl DW et al; Chemosphere 29: 523-35 (1994) (5) Hanna M; Water Pollut Res J Can 27: 833-43 (1992) (6) Hendriks AJ et al; Environ Toxicol Chem 17: 1885-98 (1998) (7) King TL et al; Bull Environ Contam Toxicol 71: 543-550 (2003)

Hazardous Substances Data Bank (HSDB)

## 11.2.19 Animal Concentrations

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1,2,4-Trichlorobenzene was detected in herring gull eggs sampled from the Detroit River in 1979, 10 pos samples at an avg 0.01 ppm; Niagara River, 10 samples, 100% pos, avg 0.02 ppm (1). Samples of Arctic fox (Alopex lagopus) muscle and liver taken from Barrow, AK, Holman, NT, and Arviat, NU had total chlorobenzene concns of 4.2-17.6 ng/g (wet weight), of which 1,2,4-trichlorobenzene is included(2). 1,2,4-Trichlorobenzene was measured in the eggs of birds in the Selenga river estuary of Lake Baikal region, Russia; (species, concn ug/kg dry weight) mallard (Anas platyrhynchos), <5; pintail (Anas acuta), 140.9; shoveler (Anas clypeata, 72.9; tufted duck (Aythya fuligula), <5; pochard (Althya ferina), <5; goose (Anser anser), <5; domestic fowl (Gallus gallus), 12.2 and 8.3; heron (Ardea cinerea), 7.2; herring gull (Larus argentatus), 23.9; common gull (Larus canus), 91.1; common tern(Sterna hirundo), <5; black headed gull (Larus ridibundus), <5; liapwing (Vanellus vanellus) 23.4; Slavonian grebe (Podiceps auritus), 7.7; marsh sandpiper (Tringa stagnatilis), 22.1(3). (1) Struger J et al; J Great Lakes Res 11; 223-30 (1985) (2) Hoekstra PF et al; Environ Pollut 122; 423-33 (2003) (3) Lebedev AT et al; Sci Total Environ 212; 153-62 (1998)

#### Hazardous Substances Data Bank (HSDB)

11.2.20 Milk Concentrations	2 (?)
ENVIRONMENTAL: 1,2,4-Trichlorobenzene was detected in human milk in Yugoslavia at a concentration of 25 ppb(1) and human milk in Canada at 0.11 ng/g (whole milk) and 3.81 ng/g (milk fat)(2). (1) Jan J; Bull Environ Contam Toxicol 30: 595-99 (1983) (2) Newsome WH et al; Chemosphere 30: 2143-53 (1995)	
Hazardous Substances Data Bank (HSDB)	
11.2.21 Other Environmental Concentrations	? Z
It has been calculated that 0.06, 0.09 and 0.288 tons of 1.2.4-trichlorobenzene are released to the air, water and soil in southern Ontario every year(1)	

PMID:10101848 (1) MacLeod M, Mackay D; Chemosphere 38: 1777-96 (1999)

Hazardous Substances Data Bank (HSDB)

11.2.22 Probable Routes of Human Exposure	0 Z

NIOSH (NOES Survey 1981-1983) has statistically estimated that 4,033 workers (1,463 of these were female) were potentially exposed to 1,2,4-trichlorobenzene in the US(1). Occupational exposure to 1,2,4-trichlorobenzene may occur through inhalation and dermal contact with this compound at workplaces where 1,2,4-trichlorobenzene is produced or used. Monitoring data indicate that the general population may be exposed to 1,2,4-trichlorobenzene via inhalation of ambient air, ingestion of food and drinking water, and dermal contact with this compound or other products containing 1,2,4-trichlorobenzene(SRC).

(1) NIOSH; NOES. National Occupational Exposure Survey conducted from 1981-1983. Estimated numbers of employees potentially exposed to specific agents by 2-digit standard industrial classification (SIC). Available from, as of July 2009: https://www.cdc.gov/noes/

Hazardous Substances Data Bank (HSDB)

#### 11.2.23 Average Daily Intake

AIR INTAKE: Estimated inhalation dosage for 1,2,4-trichlorobenzene (ug/day, based on intake of 23 cu m/day at 25 °C, 1 atm pressure), 1979: Los Angeles, CA, 11.8, Phoenix, A.Z, 4.8, Oakland, CA, 6.3(1).

(1) Singh HB et al; Atmos Measurements of Selected Toxic Organic Chem PB80-198989

## Hazardous Substances Data Bank (HSDB)

## 11.2.24 Body Burden

1,2,4-Trichlorobenzene has been detected in 26% of Canadian human adipose tissue at a mean concn of 103 ng/g(1). Combined trichlorobenzene and tetrachlorobenzene isomers were detected in human adipose tissue in Slovenia at a concn of 60 ng/g and in human hair samples at 40 ng/g(2). A 1992 epidemiologic study of 497 Canadian samples resulted in 49.1% positive detection of 1,2,4-trichlorobenzene at a median concn of 3.4 ng/g lipid with a 118 ng/g lipid maximum concn(3). 1,2,4-Trichlorobenzene was detected in 21 samples of follicular fluid, taken at the time of oocyte retrieval for in vitro fertilization at a concn of 212 pg/mL(4). 1,2,4-Trichlorobenzene was detected in human milk in Yugoslavia at a concn of 25 ppb(5) and human milk in Canada at 0.11 ng/g (whole milk) and 3.81 ng/g (milk fat)(6).

(1) Mes J et al; Bull Environ Contam Toxicol 45: 681-88 (1990) (2) Zupancic-Kralj L, Jan J; Acta Chim Slov 41: 447-56 (1994) (3) Gladen BC et al; Environ Health Perspect 11: 437-43 (2003) (4) Younglai EV et al; Arch Environ Contam Toxicol 43: 121-6 (2002) (5) Jan J; Bull Environ Contam Toxicol 30: 595-99 (1983) (6) Newsome WH et al; Chemosphere 30: 2143-53 (1995)

Hazardous Substances Data Bank (HSDB)

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Comparative Toxicogenomics Database (CTD)

13 Literature	0 Z
13.1 NLM Curated PubMed Citations	0 Z

PubChem

13.2 Springer Nature References

? Z

Springer Nature

13.3 Thieme References

0 Z

Thieme Chemistry

13.4 Wiley References

⊘ ⊿

Wiley

13.5 Depositor Provided PubMed Citations

0 Z

PubChem

13.6 Chemical Co-Occurrences in Literature

⊘⊿

PubChem

13.7 Chemical-Gene Co-Occurrences in Literature

⊘ ⊿

0 Z

PubChem

13.8 Chemical-Disease Co-Occurrences in Literature

PubChem

14 Patents	0 2
14.1 Depositor-Supplied Patent Identifiers	0 Z

PubChem

## Link to all deposited patent identifiers

PubChem

# 14.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

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

PATENTSCOPE (WIPO)

0 Z

15 Biomolecular Interactions and Pathways	0 []
15.1 Chemical-Gene Interactions	? Z
15.1.1 CTD Chemical-Gene Interactions	0 2

Comparative Toxicogenomics Database (CTD)

15.2 Pathways

?Z

PubChem

16 Biological Test Results	0 2
16.1 BioAssay Results	0 Z

PubChem

17 Classification	? Z
17.1 Ontologies	() Z
17.1.1 MeSH Tree	0 2

Medical Subject Headings (MeSH)

17.1.2 ChEBI Ontology

02

ChEBI

17.1.3 ChemIDplus

0 Z

ChemIDplus

CAMEO Chemicals

17.1.5 UN GHS Classification

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

17.1.6 EPA CPDat Classification

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02

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EPA Chemical and Products Database (CPDat)

17.1.7 NORMAN Suspect List Exchange Classification

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NORMAN Suspect List Exchange

17.1.8 EPA DSSTox Classification

EPA DSSTox

# 18 Information Sources

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1,2,4-TRICHLOROBENZENE https://cameochemicals.noaa.gov/chemical/10062 CAMEO Chemical Reactivity Classification https://cameochemicals.noaa.gov/browse/react

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1,2,4-Trichlorobenzene https://chem.nlm.nih.gov/chemidplus/sid/0000120821 Benzene, 1,2,4-trichloro-, radical ion(1-) https://chem.nlm.nih.gov/chemidplus/sid/0063697187 ChemIDplus Chemical Information Classification https://chem.nlm.nih.gov/chemidplus/

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1,2,4-Trichlorobenzene https://comptox.epa.gov/dashboard/DTXSID0021965 CompTox Chemicals Dashboard Chemical Lists https://comptox.epa.gov/dashboard/chemical\_lists/

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https://ecna.europa.eu/web/guest/iegai-not

1,2,4-trichlorobenzene

https://echa.europa.eu/substance-information/-/substanceinfo/100.004.026 1,2,4-trichlorobenzene

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/68125

0 Z

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## 8. Hazardous Substances Data Bank (HSDB)

1,2,4-TRICHLOROBENZENE https://pubchem.ncbi.nlm.nih.gov/source/hsdb/1105

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1,2,4-TRICHLOROBENZENE

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1,2,4-TRICHLOROBENZENE http://www.osha.gov/chemicaldata/chemResult.html?RecNo=161

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Benzene, 1,2,4-trichlorohttps://www.cdc.gov/niosh-rtecs/DC200B20.html 1,2,4-Trichlorobenzene

https://www.cdc.gov/niosh/npg/npgd0627.html

## 12. NJDOH RTK Hazardous Substance List

1,2,4-trichlorobenzene http://nj.gov/health/eoh/rtkweb/documents/fs/1887.pdf

#### 13. ChEBI

1,2,4-trichlorobenzene http://www.ebi.ac.uk/chebi/searchid.do?chebild=CHEBI:28222 ChEBI Ontology http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology

## 14. EPA Air Toxics

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1,2,4-Trichlorobenzene https://www.epa.gov/sites/production/files/2016-09/documents/1-2-4-trichlorobenzene.pdf

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1,2,4-trichlorobenzene https://comptox.epa.gov/dashboard/DTXSID0021965#exposure EPA CPDat Classification

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

## 17. EU REGULATION (EC) No 1272/2008

1,2,4-trichlorobenzene https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A32008R1272

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

1,2,4-trichlorobenzene http://hcis.safeworkaustralia.gov.au/HazardousChemical/Details?chemicalID=4556

## 19. NITE-CMC

1,2,4-Trichlorobenzene - FY2006 https://www.nite.go.jp/chen/english/ghs/06-imcg-0851e.html 1,2,4-Trichlorobenzene - FY2008 https://www.nite.go.jp/chen/english/ghs/08-meti-0041e.html

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## 21. NORMAN Suspect List Exchange

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1,2,4-trichlorobenzene NORMAN Suspect List Exchange Classification https://www.norman-network.com/nds/SLE/

#### 22. NMRShiftDB

https://pubchem.ncbi.nlm.nih.gov/substance/591815

#### 23. SpectraBase

1,2,4-Trichlorobenzene https://spectrabase.com/spectrum/8hSE2aD0j6l 1,2,4-Trichlorobenzene https://spectrabase.com/spectrum/6PJoFZr4MEw 1,2,4-Trichlorobenzene https://spectrabase.com/spectrum/K2lpW7WBNOL 1,2,4-TRICHLOROBENZENE https://spectrabase.com/spectrum/1N3wQS4ZbdW 1,2,4-TRICHLOROBENZENE https://spectrabase.com/spectrum/IMcCY2Pk8Le 1,2,4-TRICHLOROBENZENE https://spectrabase.com/spectrum/2omjkSTbDe4 1,2,4-TRICHLOROBENZENE https://spectrabase.com/spectrum/EyAWrWTupPh Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/7hZU6k7LzpY 1,2,4-Trichlorobenzene https://spectrabase.com/spectrum/GVPgCCFa6BI 1,2,4-TRICHLOROBENZENE https://spectrabase.com/spectrum/7eov3VKY1AO 1,2,4-TRICHLORBENZOL https://spectrabase.com/spectrum/FDi8jc86GJg PBKONEOXTCPAFI-UHFFFAOYSA-N https://spectrabase.com/spectrum/JIWT6tcqsus BENZENE, 1,2,4-TRICHLOROhttps://spectrabase.com/spectrum/4yyjCJUrGGw Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/C1m4u1Gbv0M Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/CdCZI1rgJhT Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/JVJI5wAIGYe Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/49BR00cv46M Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/44MM3bQachH Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/8BnfJrThYXM Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/8Zm3mfEHBaM Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/9rS7V5ckQNf Benzene, 1,2,4-trichloro-

https://spectrabase.com/spectrum/4P8oBZvAjU 1,2,4-trichlorobenzene https://spectrabase.com/spectrum/GuzfkwAXIXq 1.2.4-TRICHLOROBENZENE https://spectrabase.com/spectrum/79hYcPeRRMI 1,2,4-Trichlorobenzene https://spectrabase.com/spectrum/6nRTpnHNMiL 1,2,4-Trichlorobenzene https://spectrabase.com/spectrum/9opfmBmMP5H 1,2,4-Trichlorobenzene https://spectrabase.com/spectrum/3MURJHKoPGb Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/3YIX6UNUHXh Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/1Vj3RX3LzgB 1,2,4-TRICHLOROBENZENE https://spectrabase.com/spectrum/HDbvCVESW6t BENZENE, 1,2,4-TRICHLOROhttps://spectrabase.com/spectrum/LKyXwcBKNCS 1,2,4-Trichlorobenzene https://spectrabase.com/spectrum/BTNIeScCkX1 Renzene 124-trichlorohttps://spectrabase.com/spectrum/LlgprfoDFC4 Benzene, 1.2.4-trichlorohttps://spectrabase.com/spectrum/B9UG3nu1Zu6 Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/4Fa8UqZDyV6 Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/I4yNB1COQjI Benzene, 1.2.4-trichlorohttps://spectrabase.com/spectrum/GPGwABTT5SS Benzene, 1.2.4-trichlorohttps://spectrabase.com/spectrum/2KWhklD0r0S Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/8QjChwh8OSe Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/FxnaPS6PvNo Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/Hv1LixJObmy Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/CYStinQxavw Benzene, 1.2.4-trichlorohttps://spectrabase.com/spectrum/LcaXB4traro Benzene, 1,2,4-trichlorohttps://spectrabase.com/spectrum/Lw544eiOzE8

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1,2,4-TRICHLOROBENZENE http://mona.fiehnlab.ucdavis.edu/spectra/browse?inchikey=PBKONEOXTCPAFI-UHFFFAOYSA-N

#### 25. NIST Mass Spectrometry Data Center

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#### https://www.rhea-db.org/rhea?query=CHEBI:28222

# 28. Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/341150408

# 29. SpringerMaterials

1,2,4-trichloro-benzene https://materials.springer.com/substanceprofile/docs/smsid\_zulfmduaarakyjhu

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Trichlorobenzene, 1,2,4https://epa-prgs.ornl.gov/cgi-bin/chemicals/csl\_search Trichlorobenzene, 1,2,4https://epa-prgs.ornl.gov/cgi-bin/chemicals/csl\_search?tool=rml

# 32. Wikipedia

1,2,4-trichlorobenzene https://en.wikipedia.org/wiki/1,2,4-Trichlorobenzene

#### 33. Wiley

https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=181357

#### 34. PubChem

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

# 35. Medical Subject Headings (MeSH)

1,2,4-trichlorobenzene https://www.ncbi.nlm.nih.gov/mesh/67009947 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 403383350 https://pubchem.ncbi.nlm.nih.gov/substance/403383350