

# [Sym-tetrabromoethane c2h2br4 structure](https://assignbuster.com/sym-tetrabromoethane-c2h2br4-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 2 H 2 Br 4  |
| Average mass  | 345. 653 Da  |
| Density  | 3. 0±0. 1 g/cm 3  |
| Boiling Point  | 243. 5±0. 0 °C at 760 mmHg  |
| Flash Point  | 97. 0±13. 2 °C  |
| Molar Refractivity  | 42. 2±0. 3 cm 3  |
| Polarizability  | 16. 7±0. 5 10 -24 cm 3  |
| Surface Tension  | 56. 3±3. 0 dyne/cm  |
| Molar Volume  | 115. 0±3. 0 cm 3  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Predicted – Mcule
* Experimental Physico-chemical Properties

## Experimental Melting Point:

|  |
| --- |
| 0 °COxford University Chemical Safety Data (No longer updated)More details  |
| 0 °CJean-Claude Bradley Open Melting Point Dataset14723, 14889, 21161  |
| -1 °CBiosynthJ-503707  |

## Experimental Boiling Point:

|  |
| --- |
| 118-120 deg C / 15 mm (261. 7215-264. 3892 °C / 760 mmHg)Alfa Aesar  |
| 474 F (245. 5556 °C)(Decomposes)NIOSHKI8225000  |
| 135 °COxford University Chemical Safety Data (No longer updated)More details  |
| 118-120 °C / 15 mm (261. 7215-264. 3892 °C / 760 mmHg)Alfa AesarA12943  |
| 243. 5 °CBiosynthJ-503707  |

## Experimental Vapor Pressure:

|  |
| --- |
| 0. 02 mmHgNIOSHKI8225000  |

## Experimental Flash Point:

## Experimental Freezing Point:

|  |
| --- |
| 32 F (0 °C)NIOSHKI8225000  |

## Experimental Gravity:

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| --- |
| 2. 967 g/mLAlfa AesarA12943  |
| 97 g/mLBiosynthJ-503707  |

## Experimental Refraction Index:

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| --- |
| 1. 637Alfa AesarA12943  |

## Experimental Solubility:

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| --- |
| 0. 07%NIOSHKI8225000  |

* Miscellaneous

## Appearance:

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| Pale-yellow liquid with a pungent odor similar to camphor or iodoform. [Note: A solid below 32F.]NIOSHKI8225000  |
| yellowish heavy liquid with odour of camphor andOxford University Chemical Safety Data (No longer updated)More details  |

## Stability:

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| --- |
| Stable. Incompatible with strong oxidizing agents, aluminium, magnesium, alkali metals. Oxford University Chemical Safety Data (No longer updated)More details  |

## Toxicity:

|  |
| --- |
| ORL-RAT LD50 1200 mg kg-1, ORL-RBT LD50 400 mg kg-1, SKN-RAT LD50 5250 mg kg-1, IPR-MUS LD50 443 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

|  |
| --- |
| 24-27-45-61Alfa AesarA12943  |
| 26-36-52/53Alfa AesarA12943  |
| 6. 1Alfa AesarA12943  |
| DangerAlfa AesarA12943  |
| DANGER: POISON, irritates skin, eyes, lungsAlfa AesarA12943  |
| H330-H319-H412Alfa AesarA12943  |
| P260-P304+P340-P305+P351+P338-P320-P405-P501aAlfa AesarA12943  |
| Safety glasses, adequate ventilation. Oxford University Chemical Safety Data (No longer updated)More details  |
| Very Toxic/Harmful/Light SensitiveSynQuest1100-9-29  |

## First-Aid:

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| --- |
| Eye: Irrigate immediately Skin: Water flush promptly Breathing: Respiratory support Swallow: Medical attention immediatelyNIOSHKI8225000  |

## Exposure Routes:

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| inhalation, ingestion, skin and/or eye contactNIOSHKI8225000  |

## Symptoms:

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| Irritation eyes, nose; anorexia, nausea; headache; abdominal pain; jaundice; leukocytosis (increased blood leukocytes); central nervous system depressionNIOSHKI8225000  |

## Target Organs:

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| --- |
| Eyes, respiratory system, liver, central nervous systemNIOSHKI8225000  |

## Incompatibility:

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| --- |
| Strong caustics; hot iron; reducing metals such as aluminum, magnesium & zincNIOSHKI8225000  |

## Personal Protection:

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| --- |
| Skin: Prevent skin contact Eyes: Prevent eye contact Wash skin: When contaminated Remove: When wet or contaminated Change: No recommendationNIOSHKI8225000  |

## Exposure Limits:

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| --- |
| NIOSH REL : See Appendix D OSHA PEL : TWA 1 ppm (14 mg/m 3 )NIOSHKI8225000  |

* Gas Chromatography

## Retention Index (Kovats):

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| --- |
| 1277 (estimated with error: 62)NIST Spectramainlib\_341366, replib\_229884, replib\_156055  |
| 1206 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 75 C; CAS no: 79276; Active phase: OV-1; Carrier gas: He; Substrate: Chromosorb W DMCS; Data type: Kovats RI; Authors: Castello, G.; Gerbino, T. C., Effect of Temperature on the Gas Chromatographic Separation of Halogenated Compounds on Polar and Non-Polar Stationary Phases, J. Chromatogr., 437, 1988, 33-45.)NIST Spectranist ri  |
| 1226 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 100 C; CAS no: 79276; Active phase: OV-1; Carrier gas: He; Substrate: Chromosorb W DMCS; Data type: Kovats RI; Authors: Castello, G.; Gerbino, T. C., Effect of Temperature on the Gas Chromatographic Separation of Halogenated Compounds on Polar and Non-Polar Stationary Phases, J. Chromatogr., 437, 1988, 33-45.)NIST Spectranist ri  |
| 1245 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 125 C; CAS no: 79276; Active phase: OV-1; Carrier gas: He; Substrate: Chromosorb W DMCS; Data type: Kovats RI; Authors: Castello, G.; Gerbino, T. C., Effect of Temperature on the Gas Chromatographic Separation of Halogenated Compounds on Polar and Non-Polar Stationary Phases, J. Chromatogr., 437, 1988, 33-45.)NIST Spectranist ri  |
| 1265 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 150 C; CAS no: 79276; Active phase: SE-30; Carrier gas: Ar; Substrate: Gas Chrom Q (80-100 mesh); Data type: Kovats RI; Authors: Tiess, D., Gaschromatographische Retentionsindices von 125 leicht- bis mittelfluchtigen organischen Substanzen toxikologisch-analytischer Relevanz auf SE-30, Wiss. Z. Wilhelm-Pieck-Univ. Rostock Math. Naturwiss. Reihe, 33, 1984, 6-9.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1268. 5 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 2 mm; Column length: 50 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 20 C; End T: 200 C; Start time: 5 min; CAS no: 79276; Active phase: Methyl Silicone; Carrier gas: N2; Data type: Normal alkane RI; Authors: Yasuhara, A.; Morita, M.; Fuwa, K., Temperature-programmed retention indices of 221 halogenated organic compounds with 1-bromoalkanes as references, J. Chromatogr., 328, 1985, 35-48.)NIST Spectranist ri  |

Predicted data is generated using the ACD/Labs Percepta Platform – PhysChem Module

|  |  |
| --- | --- |
| Density:  | 3. 0±0. 1 g/cm 3  |
| Boiling Point:  | 243. 5±0. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 1±0. 4 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 46. 1±3. 0 kJ/mol  |
| Flash Point:  | 97. 0±13. 2 °C  |
| Index of Refraction:  | 1. 654  |
| Molar Refractivity:  | 42. 2±0. 3 cm 3  |
| #H bond acceptors:  | 0  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 1  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 4. 12  |
| ACD/LogD (pH 5. 5):  | 3. 59  |
| ACD/BCF (pH 5. 5):  | 315. 62  |
| ACD/KOC (pH 5. 5):  | 2140. 46  |
| ACD/LogD (pH 7. 4):  | 3. 59  |
| ACD/BCF (pH 7. 4):  | 315. 62  |
| ACD/KOC (pH 7. 4):  | 2140. 46  |
| Polar Surface Area:  | 0 Å 2  |
| Polarizability:  | 16. 7±0. 5 10 -24 cm 3  |
| Surface Tension:  | 56. 3±3. 0 dyne/cm  |
| Molar Volume:  | 115. 0±3. 0 cm 3  |

Predicted data is generated using the US Environmental Protection Agency’s EPISuite™

 Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 2. 55Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 238. 93 (Adapted Stein & Brown method)Melting Pt (deg C): 37. 10 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0614 (Mean VP of Antoine & Grain methods)MP (exp database): 0 deg CBP (exp database): 243. 5 deg CVP (exp database): 2. 00E-02 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 43. 66log Kow used: 2. 55 (estimated)no-melting pt equation usedWater Sol (Exper. database match) = 678 mg/L (25 deg C)Exper. Ref: HORVATH, AL ET AL. (1999)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 285. 43 mg/LWat Sol (Exper. database match) = 678. 00Exper. Ref: HORVATH, AL ET AL. (1999)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 72E-005 atm-m3/moleGroup Method: IncompleteExper Database: 1. 40E-05 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 6. 396E-004 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 55 (KowWin est)Log Kaw used: -3. 242 (exp database)Log Koa (KOAWIN v1. 10 estimate): 5. 792Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 3983Biowin2 (Non-Linear Model) : 0. 0000Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 5511 (weeks-months)Biowin4 (Primary Survey Model) : 3. 4906 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : -0. 0305Biowin6 (MITI Non-Linear Model): 0. 0001Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 1. 9407Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 2. 67 Pa (0. 02 mm Hg)Log Koa (Koawin est ): 5. 792Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 13E-006 Octanol/air (Koa) model: 1. 52E-007 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 4. 06E-005 Mackay model : 9E-005 Octanol/air (Koa) model: 1. 22E-005 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 1399 E-12 cm3/molecule-secHalf-Life = 76. 439 Days (12-hr day; 1. 5E6 OH/cm3)Ozone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 6. 53E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 106. 8Log Koc: 2. 029 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 3. 064E+003 L/mol-secKb Half-Life at pH 8: 3. 770 minutesKb Half-Life at pH 7: 37. 697 minutesBioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 1. 264 (BCF = 18. 36)log Kow used: 2. 55 (estimated)Volatilization from Water: Henry LC: 1. 4E-005 atm-m3/mole (Henry experimental database)Half-Life from Model River: 79. 65 hours (3. 319 days)Half-Life from Model Lake : 1025 hours (42. 7 days)Removal In Wastewater Treatment: Total removal: 3. 99 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 3. 13 percentTotal to Air: 0. 76 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 3. 62 1. 83e+003 1000 Water 21. 8 900 1000 Soil 74. 4 1. 8e+003 1000 Sediment 0. 196 8. 1e+003 0 Persistence Time: 954 hr

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* 1-Click Scaffold Hop