Sym-tetrabromoethane c2h2br4 structure

ASSIGN BUSTER

Contents

- Retention Index (Normal Alkane):

Molecular Formula	$C_2H_2Br_4$
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)NIOSHKI82250

00

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:**

  2. 967 g/mLAlfa

  AesarA12943

  97 g/mLBiosynthJ-503707

- **Experimental Refraction Index:**

  1. 637Alfa

  AesarA12943

- **Experimental Solubility:**

  0.

07%NIOSHKI8225000

- Miscellaneous

- **Appearance:**

  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  yellowish heavy liquid with odour of camphor andOxford University Chemical Safety Data (No longer updated)More details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:**

  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 Oxford University Chemical Safety Data (No longer updated)More details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:**

  Eye: Irrigate immediately

  Skin: Water flush promptly

  Breathing: Respiratory

  support Swallow: Medical

  attention

  immediatelyNIOSHKI822500

  0

- **Exposure Routes:**

  inhalation, ingestion, skin

  and/or eye

  contactNIOSHKI8225000

- **Symptoms:**

  Irritation eyes, nose;

  anorexia, nausea; headache;

  abdominal pain; jaundice;

  leukocytosis (increased

  blood leukocytes); central

  nervous system

  depressionNIOSHKI8225000

- **Target Organs:**

  Eyes, respiratory system,

  liver, central nervous

  systemNIOSHKI8225000

- **Incompatibility:**

  Strong caustics; hot iron;

  reducing metals such as

  aluminum, magnesium &

  zincNIOSHKI8225000

- **Personal Protection:**

  Skin: Prevent skin contact

  Eyes: Prevent eye contact

  Wash skin: When

  contaminated Remove:

  When wet or contaminated

Change: No

recommendationNIOSHKI822

5000

- **Exposure Limits:**

  NIOSH REL : See Appendix D

  OSHA PEL : TWA 1 ppm (14

  mg/m 3)NIOSHKI8225000

- Gas Chromatography

  - **Retention Index (Kovats):**

    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

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop