Boric acid h3bo3 structure

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- Bio Activity:

Molecular Formula	H_3BO_3
Average mass	61. 833 Da
Density	1. 4±0. 1 g/cm^3
Boiling Point	
Flash Point	
Molar Refractivity	10. 1±0. 3 cm^3
Polarizability	4. 0±0. 5 10^{-24}

	cm ^{3}
Surface Tension	59. 2±3. 0 dyne/cm
Molar Volume	43. 0±3. 0 cm ^{3}

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

Experimental Melting Point:

185 °C (Decomposes)Alfa Aesar33253, 12680, 10659

170. 9 °CJean-Claude Bradley Open Melting Point Dataset20629

185 °C (Decomposes)Alfa Aesar36771, A16624, A10896

160 °C (Decomposes)Oakwood094443

170. 9 °CLabNetworkLN00193674

171 °CFooDBFDB014459

- **Experimental Flash Point:**
- **Experimental Gravity:**

  1. 435 g/mLAlfa Aesar36771, A16624, A10896

  1. 44 g/mLOakwood094443

  1. 44 g/mLFluorochem

  1. 44 g/lFluorochem094443

- **Experimental Solubility:**

  Soluble in water (1 gram in 18ml cold or 4ml boiling water). Solubility in w increased by addition of HCl, citric or tartaric acidAlfa Aesar33253

  Soluble to 600 mM in waterTocris Bioscience3177

- Miscellaneous

- **Safety:**

  53-45Alfa AesarA10896, A16624, 36771

  60-61Alfa AesarA10896, A16624, 36771

  DangerAlfa AesarA10896, A16624

  H360FDAlfa AesarA10896, A16624

  P201-P308+P313Alfa AesarA10896, A16624

TAbblis ChemicalsAB1002298

WARNING: Irreversible damage risk, protect skin/eyes/lungs. Alfa AesarA

A16624, 10659, 12680, 33253, 36771

WARNING: Irritates eyes, lungs, may be harmful if swallowedAlfa AesarA

A16624, 10659, 12680, 33253, 36771

- **Bio Activity:**

Buffers, Solvents and SolutionsTocris

Bioscience3177

ReagentsTocris Bioscience3177

Widely used in buffers for electrophoresisTocris

Bioscience3177

Widely used in buffers for electrophoresis. Tocris

Bioscience3177

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

PhysChem Module

Density: 1. 4±0. 1 g/cm ^{3}

Boiling Point:

Vapour Pressure:

Enthalpy of Vaporization:	
Flash Point:	
Index of Refraction:	1. 385
Molar Refractivity:	10. 1±0. 3 cm^3
#H bond acceptors:	3
#H bond donors:	3
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	0
ACD/LogP:	-0. 29
ACD/LogD (pH 5. 5):	
ACD/BCF (pH 5. 5):	
ACD/KOC (pH 5. 5):	
ACD/LogD (pH 7. 4):	
ACD/BCF (pH 7. 4):	
ACD/KOC (pH 7. 4):	
Polar Surface Area:	61 $Å^2$

Polarizability: $4.0 \pm 0.5\ 10^{-24}\ cm^3$

Surface Tension: 59. 2±3. 0 dyne/cm

Molar Volume: $43.0 \pm 3.0\ cm^3$

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

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = -0. 22Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 616. 55 (Adapted Stein & Brown method)Melting Pt (deg C): 267. 04 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 7. 36E-017 (Modified Grain method)MP (exp database): 170. 9 deg CSubcooled liquid VP: 2. 37E-015 mm Hg (25 deg C, Mod-Grain method)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 2. 117e+005log Kow used: -0. 22 (estimated)no-melting pt equation usedWater Sol (Exper. database match) = 5e+004 mg/L (25 deg C)Exper. Ref: SHIU, WY ET AL. (1990)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1e+006 mg/LWat Sol (Exper. database match) = 50000. 00Exper. Ref: SHIU, WY ET AL. (1990)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : IncompleteGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 2. 828E-023 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Can Not Estimate (can not calculate HenryLC)Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7181Biowin2 (Non-Linear Model) : 0. 8938Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 0625 (weeks)Biowin4 (Primary Survey Model) : 3. 7585 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5282Biowin6 (MITI Non-Linear Model): 0. 6771Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 8361Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C) [AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 3. 16E-013 Pa (2. 37E-015 mm Hg)Log Koa (): not availableKp (particle/gas partition coef. (m3/ug)): Mackay model : 9. 49E+006 Octanol/air (Koa) model: not availableFraction sorbed to airborne particulates (phi): Junge-Pankow model : 1 Mackay model : 1 Octanol/air (Koa) model: not availableAtmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 4200 E-12 cm3/molecule-secHalf-Life = 25. 467 Days (12-hr day; 1. 5E6 OH/cm3)Ozone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 1 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 35. 04Log Koc: 1. 545 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Rate constants can NOT be estimated for this structure! Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 0. 500 (BCF = 3. 162)log Kow used: -0. 22 (estimated)Volatilization from Water: Henry LC: 2. 83E-023 atm-m3/mole (calculated from VP/WS)Half-Life from Model River: 1. 628E+019 hours (6. 782E+017 days)Half-Life from Model Lake : 1. 776E+020 hours (7. 399E+018

days)Removal In Wastewater Treatment: Total removal: 1. 85 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 76 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 3. 28e-008 611 1000 Water 38. 7 360 1000 Soil 61. 2 720 1000 Sediment 0. 0711 3. 24e+003 0 Persistence Time: 581 hr

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