2,2-bis(hydroxymethyl)propionic acid c5h10o4 structure

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Molecular Formula	$C_5H_{10}O_4$
Average mass	134. 130 Da
Density	1. 3±0. 1 g/cm ^{3}
Boiling Point	366. 7±32. 0 °C at 760 mmHg
Flash Point	189. 7±21. 6 °C

Molar Refractivity	29. 8±0. 3 cm^3
Polarizability	11. 8±0. 5 10^{-24} cm^3
Surface Tension	60. 9±3. 0 dyne/cm
Molar Volume	100. 8±3. 0 cm^3

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

Experimental Melting Point:

189-191 °CSynQuest

185 °CTCIB1192

182-186 °CMerck

Millipore2239, 814996

189 °CJean-Claude

Bradley Open Melting

Point Dataset1117

190 °CJean-Claude

Bradley Open Melting

Point Dataset24047

187-191 °CAlfa

AesarL14014

189-191

°CSynQuest52269,

2129-1-22

187-191

°COakwood[241292]

190 °CBiosynthQ-

200158

187-191

°CLabNetworkLN00142

406

- **Experimental Boiling Point:**

  219 °CBiosynthJ-

  660014, J-660058

- **Experimental LogP:**

  -1. 898Vitas-

  MSTL146614

- **Experimental Flash Point:**

  150 °CBiosynthQ-

  200158

  150

  °CLabNetworkLN00142

  406

- **Experimental Gravity:**

  150 g/mLBiosynthQ-

  200158

  95. 6 g/mLBiosynthJ-

  660014, J-660058

- Predicted Physico-chemical Properties

  - **Predicted Melting Point:**

    185 °CTCI

    185

    °CTCIB1192

- Miscellaneous

- **Appearance:**

  White powderNovochemy[NC-

  30410]

- **Safety:**

  20/21/36/37/39Novoch

  emy[NC-30410]

  26-37Alfa AesarL14014

  26-37-60Alfa

  AesarL14014

  36/37/38Alfa

  AesarL14014

  36/37/38Novochemy[N

  C-30410]

  GHS07BiosynthQ-

  200158

  GHS07;

  GHS09Novochemy[NC-

  30410]

  H304;

  H403Novochemy[NC-

30410]

H315; H319;

H335BiosynthQ-

200158

H315-H319-H335Alfa

AesarL14014

IRRITANTAlfa

AesarL14014

IrritantSynQuest2129-

1-22, 52269

P102; P210; P262;

P270; P302+P352;

P308+P313Novochemy

[NC-30410]

P261; P280;

P302+P352;

P304+P340;

P305+P351+P338;

P312BiosynthQ-200158

P261-P280-

P305+P351+P338-

P304+P340-P405-

P501aAlfa AesarL14014

R22Novochemy[NC-

30410]

R36/37/38SynQuest212

9-1-22, 52269

S26SynQuest2129-1-

22, 52269

WarningAlfa

AesarL14014

WarningBiosynthQ-

200158

WarningNovochemy[NC

-30410]

- Gas Chromatography

- **Retention Index (Kovats):**

  1276 (estimated with

  error: 89)NIST

  Spectramainlib_235948

  , replib_160016

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

Density:	1. 3±0. 1 g/cm ^{3}
Boiling Point:	366. 7±32. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±1. 9 mmHg at 25°C
Enthalpy of Vaporization:	71. 0±6. 0 kJ/mol
Flash Point:	189. 7±21. 6 °C
Index of Refraction:	1. 504
Molar Refractivity:	29. 8±0. 3 cm ^{3}
#H bond acceptors:	4
#H bond donors:	3
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	0
ACD/LogP:	-1. 90
ACD/LogD (pH 5. 5):	-2. 72
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	1. 00

ACD/LogD (pH 7. 4):	-4. 47
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	1. 00
Polar Surface Area:	78 Å ^{2}
Polarizability:	11. 8±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	60. 9±3. 0 dyne/cm
Molar Volume:	100. 8±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) = -1. 07Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 301. 50 (Adapted Stein & Brown method)Melting Pt (deg C): 86. 19 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 24E-006 (Modified Grain method)MP (exp database): 190 deg CSubcooled liquid VP: 6. 65E-005 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): 1e+006log Kow used: -1. 07 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1e+006 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral Organics-acidHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 71E-012 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 2. 188E-013 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -1. 07 (KowWin est)Log Kaw used: -10. 155 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 9. 085Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8899Biowin2 (Non-Linear Model) : 0. 9055Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 3752 (days-weeks)Biowin4 (Primary Survey Model) : 4. 1452 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 9834Biowin6 (MITI Non-Linear Model): 0. 9558Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 9266Ready 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): 0. 00887 Pa (6. 65E-005 mm Hg)Log Koa (Koawin est): 9. 085Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 000338 Octanol/air (Koa) model: 0. 000299 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 0121 Mackay model : 0. 0264 Octanol/air (Koa) model: 0. 0233 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 9. 0090 E-12 cm3/molecule-secHalf-Life = 1. 187 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 14. 247 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 0192 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1Log Koc: 0. 000 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: -1. 07 (estimated)Volatilization from Water: Henry LC: 1. 71E-012 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 3. 965E+008 hours (1. 652E+007 days)Half-Life from Model Lake : 4. 326E+009 hours (1. 802E+008 days)Removal In Wastewater Treatment: Total removal: 1. 85 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 75 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 7. 11e-005 28. 5 1000 Water 34. 4 208 1000 Soil 65. 5 416 1000 Sediment 0. 0596 1. 87e+003 0 Persistence Time: 387 hr

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- 1-Click Docking
- 1-Click Scaffold Hop