

# [2,2-bis(hydroxymethyl)propionic acid c5h10o4 structure](https://assignbuster.com/22-bishydroxymethylpropionic-acid-c5h10o4-structure/)

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* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula  | C 5 H 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 °CLabNetworkLN00142406  |

## Experimental Boiling Point:

|  |
| --- |
| 219 °CBiosynthJ-660014, J-660058  |

## Experimental LogP:

|  |
| --- |
| -1. 898Vitas-MSTL146614  |

## Experimental Flash Point:

|  |
| --- |
| 150 °CBiosynthQ-200158  |
| 150 °CLabNetworkLN00142406  |

## 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:

|  |
| --- |
| 20/21/36/37/39Novochemy[NC-30410]  |
| 26-37Alfa AesarL14014  |
| 26-37-60Alfa AesarL14014  |
| 36/37/38Alfa AesarL14014  |
| 36/37/38Novochemy[NC-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]  |
| R36/37/38SynQuest2129-1-22, 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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