

# [Diethyl cyanophosphonate c5h10no3p structure](https://assignbuster.com/diethyl-cyanophosphonate-c5h10no3p-structure/)

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* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula | C 5 H 10 NO 3 P |
| Average mass | 163. 112 Da |
| Density | 1. 2±0. 1 g/cm 3 |
| Boiling Point | 214. 2±9. 0 °C at 760 mmHg |
| Flash Point | 80. 6±0. 0 °C |
| Molar Refractivity | 35. 5±0. 3 cm 3 |
| Polarizability | 14. 1±0. 5 10 -24 cm 3 |
| Surface Tension | 38. 0±3. 0 dyne/cm |
| Molar Volume | 141. 3±3. 0 cm 3 |

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

## Experimental Boiling Point:

|  |
| --- |
| 104-105 °C / 19 mm (234. 8649-236. 18 °C / 760 mmHg)Alfa AesarL14107 |
| 104-105 °C / 19 mmHg (234. 8649-236. 18 °C / 760 mmHg)SynQuest57748, 8177-1-X0 |
| 104-105 C / 19 mmHg (234. 8649-236. 18 °C / 760 mmHg)(Literature)LabNetworkLN00848328 |

## Experimental Flash Point:

|  |
| --- |
| 80 °CAlfa Aesar |
| 80 °F (26. 6667 °C)Alfa AesarL14107 |
| 80 °CSynQuest57748, 8177-1-X0 |
| 81 °CLabNetworkLN00848328 |

## Experimental Gravity:

|  |
| --- |
| 1. 075 g/mLAlfa AesarL14107 |
| 1. 075 g/mLSynQuest8177-1-X0 |

## Experimental Refraction Index:

|  |
| --- |
| 1. 401Alfa AesarL14107 |

* Miscellaneous

## Safety:

|  |
| --- |
| 26/27/28-34Alfa AesarL14107 |
| 26-28-36/37/39-45Alfa AesarL14107 |
| 8Alfa AesarL14107 |
| Corrosive/Very Toxic/Stench/Moisture Sensitive/Store under Argon/Keep ColdSynQuest57748, 8177-1-X0 |
| DangerAlfa AesarL14107 |
| DANGER: CORROSIVE, POISON, irritates skin and eyesAlfa AesarL14107 |
| H300-H310-H330-H314Alfa AesarL14107 |
| P280-P305+P351+P338-P304+P340-P309-P310-P302+P352Alfa AesarL14107 |

* Gas Chromatography

## Retention Index (Linear):

|  |
| --- |
| 1046 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 40 C; End T: 280 C; End time: 10 min; Start time: 1 min; CAS no: 2942587; Active phase: SE-54; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Kostiainen, O., Gas Chromatography in Screening of Chemicals Related to the Chemical Weapons Convention, in Encyclopedia of Analytical Chemistry, Meyers, R. A., ed(s), John Wiley & Sons Ltd, Chichester, 2000, 963-979.)NIST Spectranist ri |

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

|  |  |
| --- | --- |
| Density: | 1. 2±0. 1 g/cm 3 |
| Boiling Point: | 214. 2±9. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 2±0. 4 mmHg at 25°C |
| Enthalpy of Vaporization: | 45. 1±3. 0 kJ/mol |
| Flash Point: | 80. 6±0. 0 °C |
| Index of Refraction: | 1. 416 |
| Molar Refractivity: | 35. 5±0. 3 cm 3 |
| #H bond acceptors: | 4 |
| #H bond donors: | 0 |
| #Freely Rotating Bonds: | 5 |
| #Rule of 5 Violations: | 0 |

|  |  |
| --- | --- |
| ACD/LogP: | 0. 04 |
| ACD/LogD (pH 5. 5): | 0. 19 |
| ACD/BCF (pH 5. 5): | 1. 00 |
| ACD/KOC (pH 5. 5): | 30. 03 |
| ACD/LogD (pH 7. 4): | 0. 19 |
| ACD/BCF (pH 7. 4): | 1. 00 |
| ACD/KOC (pH 7. 4): | 30. 03 |
| Polar Surface Area: | 69 Å 2 |
| Polarizability: | 14. 1±0. 5 10 -24 cm 3 |
| Surface Tension: | 38. 0±3. 0 dyne/cm |
| Molar Volume: | 141. 3±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. 65Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 267. 71 (Adapted Stein & Brown method)Melting Pt (deg C): 29. 34 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00975 (Modified Grain method)Subcooled liquid VP: 0. 0107 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): 1. 846e+004log Kow used: 0. 65 (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: EstersEsters (phosphate)Henrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 6. 95E-007 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 134E-007 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 65 (KowWin est)Log Kaw used: -4. 546 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 5. 196Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6699Biowin2 (Non-Linear Model) : 0. 6665Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 8387 (weeks )Biowin4 (Primary Survey Model) : 3. 6124 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3265Biowin6 (MITI Non-Linear Model): 0. 2166Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 7289Ready 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): 1. 43 Pa (0. 0107 mm Hg)Log Koa (Koawin est ): 5. 196Kp (particle/gas partition coef. (m3/ug)): Mackay model : 2. 1E-006 Octanol/air (Koa) model: 3. 85E-008 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 7. 59E-005 Mackay model : 0. 000168 Octanol/air (Koa) model: 3. 08E-006 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 38. 6286 E-12 cm3/molecule-secHalf-Life = 0. 277 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 3. 323 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 000122 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 26Log Koc: 1. 415 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. 65 (estimated)Volatilization from Water: Henry LC: 6. 95E-007 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1077 hours (44. 88 days)Half-Life from Model Lake : 1. 186E+004 hours (494. 1 days)Removal In Wastewater Treatment: Total removal: 1. 90 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 77 percentTotal to Air: 0. 04 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 865 6. 65 1000 Water 45. 7 360 1000 Soil 53. 3 720 1000 Sediment 0. 0872 3. 24e+003 0 Persistence Time: 352 hr

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