Diethyl cyanophosphonate c5h10no3p structure

\n[toc title="Table of Contents"]\n

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Contents

Molecular Formula	$C_5H_{10}NO_3P$
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)LabNetwork

LN00848328

- **Experimental Flash Point:**

80 °CAlfa Aesar

80 °F (26. 6667 °C)Alfa

AesarL14107

80 °CSynQuest57748,

8177-1-X0

81

°CLabNetworkLN00848

328

- **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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- 1-Click Scaffold Hop