Trimethyl phosphite c3h9o3p structure

Contents

Molecular Formula	$C_3H_9O_3P$
Average mass	124. 076 Da
Density	
Boiling Point	110. 2±8. 0 °C at 760 mmHg
Flash Point	27. 8±0. 0 °C
Molar Refractivity	
Polarizability	
Surface Tension	
Molar Volume	

- **Experimental Melting Point:**

  -78 °CAlfa Aesar

  110-112 °COxford University Chemical Safety Data (No longer updated)More details

  -78 °CJean-Claude Bradley Open Melting Point Dataset20234, 8645

  -78 °CAlfa Aesar30132, 43988

  -78 °CLabNetworkLN00192882

- **Experimental Boiling Point:**

  111-112 °CAlfa Aesar

  232 F (111. 1111 °C)NIOSHTH1400000

  111-112 °CAlfa Aesar30132, 43988

  111-112 °COakwood080270

  111-112 °CLabNetworkLN00192882

- **Experimental Flash Point:**

  82 F (27. 7778

°C)NIOSHTH1400000

27 °CAlfa Aesar

27 °F (-2. 7778 °C)Alfa Aesar30132,

43988

28 °COakwood080270

82 °CLabNetworkLN00192882

- **Experimental Freezing Point:**

  -108 F (-77. 7778

  °C)NIOSHTH1400000

- **Experimental Gravity:**

  20 g/mLMerck Millipore1820

  20 g/lMerck Millipore1820,

  800553

  1. 052 g/mLAlfa Aesar30132,

  43988

  1. 052 g/mLOakwood080270

- **Experimental Refraction Index:**

  1. 408Alfa Aesar43988,

30132

- **Experimental Solubility:**

  ReactsNIOSHTH14000

  00

- Miscellaneous

  - **Appearance:**

    Colorless liquid with a distinctive, pungent odor. NIOSHTH1400000

    liquid with a very unpleasant smellOxford University Chemical Safety Da

    longer updated)More details

  - **Stability:**

    Stable. Flammable. Incompatible with strong oxidizing agents, strong ba

    Moisture and air sensitive. Oxford University Chemical Safety Data (No l

    updated)More details

  - **Toxicity:**

    ORL-RAT LD50 1600 mg kg-1, IPR-RAT LD50 4180 mg kg-1, SKN-RBT LD5

    mg kg-1Oxford University Chemical Safety Data (No longer updated)Mor

  - **Safety:**

    10-22-36/37/38-63Alfa Aesar30132, 43988

    23-26-36/37Alfa Aesar30132

23-26-36/37-60Alfa Aesar30132, 43988

3Alfa Aesar30132, 43988

DANGER: FLAMMABLE, causes CNS effects, irritates skin & eyesAlfa Aesa

43988

H226-H361-H302-H315-H319-H335Alfa Aesar30132, 43988

P210-P261-P303+P361+P353-P305+P351+P338-P405-P501aAlfa Aesar3

43988

Safety glasses, gloves, good ventilation. Oxford University Chemical Safe

(No longer updated)More details

WarningAlfa Aesar30132, 43988

- **First-Aid:**

  Eye: Irrigate immediately Skin: Soap flush immediately Breathing: Respir

  support Swallow: Medical attention immediatelyNIOSHTH1400000

- **Exposure Routes:**

  inhalation, ingestion, skin and/or eye

  contactNIOSHTH1400000

- **Symptoms:**

  Irritation eyes, skin, upper respiratory system; dermatitis; in animals: ter

effectsNIOSHTH1400000

- **Target Organs:**

  Eyes, skin, respiratory system, reproductive systemNIOSHTH1400000

- **Incompatibility:**

  Magnesium perchlorate, water [Note: Reacts (hydrolyzes) with water.]NIOSHTH1400000

- **Personal Protection:**

  Skin: Prevent skin contact Eyes: Prevent eye contact Wash skin: When contaminated Remove: When wet (flammable) Change: No recommenda Provide: Quick drenchNIOSHTH1400000

- **Exposure Limits:**

  NIOSH REL : TWA 2 ppm (10 mg/m 3) OSHA PEL ?: noneNIOSHTH1400000

- Gas Chromatography

  - **Retention Index (Kovats):**

    674 (estimated with error: 89)NIST Spectramainlib_229590, replib_160241, replib_69509

  - **Retention Index (Normal Alkane):**

    688 (Program type: Complex; Column... (show more)class: Semi-standar

polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C
Description: 45 0C (2 min) ^ 8 0C/min -> 125 0C ^ 15 0C/min -> 280 0C
no: 121459; Active phase: DB-5 MS; Carrier gas: Helium; Phase thickness
um; Data type: Normal alkane RI; Authors: Tsunoda, N., The sarin incider
Japan and mass spectrometry, J. MAss Spectrom. Soc. Japan, 53(3), 2005
163.)NIST Spectranist ri

- **Retention Index (Linear):**

  689 (Program type: Ramp; Column cl… (show more)ass: Semi-standard n
  polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: C
  Heat rate: 10 K/min; Start T: 40 C; End T: 280 C; End time: 10 min; Start
  min; CAS no: 121459; Active phase: SE-54; Carrier gas: He; Phase thickn
  25 um; Data type: Linear RI; Authors: Kostiainen, O., Gas Chromatograph
  Screening of Chemicals Related to the Chemical Weapons Convention, in
  Encyclopedia of Analytical Chemistry, Meyers, R. A., ed(s), John Wiley & S
  Chichester, 2000, 963-979.)NIST Spectranist ri

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

Density:	
Boiling Point:	110. 2±8. 0 °C at 760 mmHg
Vapour Pressure:	28. 1±0. 2 mmHg at 25°C
Enthalpy of Vaporization:	33. 4±3. 0 kJ/mol

Flash Point:	27. 8±0. 0 °C
Index of Refraction:	
Molar Refractivity:	
#H bond acceptors:	3
#H bond donors:	0
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	0
ACD/LogP:	-0. 93
ACD/LogD (pH 5. 5):	-0. 09
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	21. 24
ACD/LogD (pH 7. 4):	-0. 09
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	21. 24
Polar Surface Area:	41 Å ^{2}
Polarizability:	

Surface Tension:

Molar Volume:

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. 73Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 115. 91 (Adapted Stein & Brown method)Melting Pt (deg C): -57. 62 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 22. 8 (Mean VP of Antoine & Grain methods)BP (exp database): 111. 5 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 4. 065e+005log Kow used: -0. 73 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1702. 6 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 07E-005 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 9. 157E-006 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -0. 73 (KowWin est)Log Kaw used: -3. 359 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 2. 629Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6885Biowin2 (Non-Linear Model) : 0. 7767Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 9250 (weeks)Biowin4 (Primary Survey Model) : 3. 6687 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3442Biowin6 (MITI Non-Linear Model): 0. 2693Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 5974Ready 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): 2. 85E+003 Pa (21. 4 mm Hg)Log Koa (Koawin est): 2. 629Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 05E-009 Octanol/air (Koa) model: 1. 04E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 3. 8E-008 Mackay model : 8. 41E-008 Octanol/air (Koa) model: 8. 36E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 8. 3640 E-12 cm3/molecule-secHalf-Life = 1. 279 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 15. 346 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 6. 1E-008 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 252. 8Log Koc: 2. 403 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. 73 (estimated)Volatilization from Water: Henry LC: 1. 07E-005 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 62. 09 hours (2. 587 days)Half-Life from Model Lake : 770. 7 hours (32. 11 days)Removal In Wastewater Treatment: Total removal: 2. 43 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 75 percentTotal to Air: 0. 60 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 3. 65 30. 7 1000 Water 47. 5 360

1000 Soil 48. 8 720 1000 Sediment 0. 0869 3. 24e+003 0 Persistence Time: 328 hr