

# [Trimethyl phosphite c3h9o3p structure](https://assignbuster.com/trimethyl-phosphite-c3h9o3p-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula | C 3 H 9 O 3 P |
| 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 data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Experimental Physico-chemical Properties

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| 110-112 °COxford University Chemical Safety Data (No longer updated)More details |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

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| --- |
| -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:

|  |
| --- |
| ReactsNIOSHTH1400000 |

* Miscellaneous

## Appearance:

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| Colorless liquid with a distinctive, pungent odor. NIOSHTH1400000 |
| liquid with a very unpleasant smellOxford University Chemical Safety Data (No longer updated)More details |

## Stability:

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| Stable. Flammable. Incompatible with strong oxidizing agents, strong bases. Moisture and air sensitive. Oxford University Chemical Safety Data (No longer updated)More details |

## Toxicity:

|  |
| --- |
| ORL-RAT LD50 1600 mg kg-1, IPR-RAT LD50 4180 mg kg-1, SKN-RBT LD50 2600 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details |

## 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 Aesar30132, 43988 |
| H226-H361-H302-H315-H319-H335Alfa Aesar30132, 43988 |
| P210-P261-P303+P361+P353-P305+P351+P338-P405-P501aAlfa Aesar30132, 43988 |
| Safety glasses, gloves, good ventilation. Oxford University Chemical Safety Data (No longer updated)More details |
| WarningAlfa Aesar30132, 43988 |

## First-Aid:

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| --- |
| Eye: Irrigate immediately Skin: Soap flush immediately Breathing: Respiratory support Swallow: Medical attention immediatelyNIOSHTH1400000 |

## Exposure Routes:

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| inhalation, ingestion, skin and/or eye contactNIOSHTH1400000 |

## Symptoms:

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| --- |
| Irritation eyes, skin, upper respiratory system; dermatitis; in animals: teratogenic 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 recommendation Provide: Quick drenchNIOSHTH1400000 |

## Exposure Limits:

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

* Gas Chromatography

## Retention Index (Kovats):

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| --- |
| 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-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 45 0C (2 min) ^ 8 0C/min -> 125 0C ^ 15 0C/min -> 280 0C; CAS no: 121459; Active phase: DB-5 MS; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Tsunoda, N., The sarin incidents in Japan and mass spectrometry, J. MAss Spectrom. Soc. Japan, 53(3), 2005, 157-163.)NIST Spectranist ri |

## Retention Index (Linear):

|  |
| --- |
| 689 (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: 121459; 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: |  |
| 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