

# [1,1,2,3-tetrachloro-1-propene c3h2cl4 structure](https://assignbuster.com/1123-tetrachloro-1-propene-c3h2cl4-structure/)

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

\n \t

1. [Experimental Boiling Point:](#experimental-boiling-point) \n \t
2. [Experimental Gravity:](#experimental-gravity) \n \t
3. [Experimental Refraction Index:](#experimental-refraction-index) \n \t
4. [Safety:](#safety) \n \t
5. [Retention Index (Kovats):](#retention-index-kovats) \n

\n[/toc]\n \n

Contents

* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula | C 3 H 2 Cl 4 |
| Average mass | 179. 860 Da |
| Density | 1. 5±0. 1 g/cm 3 |
| Boiling Point | 173. 8±35. 0 °C at 760 mmHg |
| Flash Point | 62. 3±23. 3 °C |
| Molar Refractivity | 35. 1±0. 3 cm 3 |
| Polarizability | 13. 9±0. 5 10 -24 cm 3 |
| Surface Tension | 35. 4±3. 0 dyne/cm |
| Molar Volume | 116. 8±3. 0 cm 3 |

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

## Experimental Boiling Point:

|  |
| --- |
| 162 °C / 743 mmHg (162. 9321 °C / 760 mmHg)SynQuest63457, 1300-5-08 |

## Experimental Gravity:

|  |
| --- |
| 20 g/mLSynQuest1300-5-08 |
| 1. 5498 g/mLSynQuest1300-5-08 |

## Experimental Refraction Index:

|  |
| --- |
| 1. 5202SynQuest63457, 1300-5-08 |

* Miscellaneous

## Safety:

|  |
| --- |
| R23/24/25, R36/38, R43SynQuest1300-5-08, 63457 |
| S3/7, S13, S23, S24/25, S26, S36/37/39, S45SynQuest1300-5-08, 63457 |
| Toxic/Irritant/Skin sensitizerSynQuest1300-5-08, 63457 |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1035 (estimated with error: 72)NIST Spectramainlib\_115038 |

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

|  |  |
| --- | --- |
| Density: | 1. 5±0. 1 g/cm 3 |
| Boiling Point: | 173. 8±35. 0 °C at 760 mmHg |
| Vapour Pressure: | 1. 7±0. 3 mmHg at 25°C |
| Enthalpy of Vaporization: | 39. 3±3. 0 kJ/mol |
| Flash Point: | 62. 3±23. 3 °C |
| Index of Refraction: | 1. 513 |
| Molar Refractivity: | 35. 1±0. 3 cm 3 |
| #H bond acceptors: | 0 |
| #H bond donors: | 0 |
| #Freely Rotating Bonds: | 1 |
| #Rule of 5 Violations: | 0 |

|  |  |
| --- | --- |
| ACD/LogP: | 3. 49 |
| ACD/LogD (pH 5. 5): | 3. 44 |
| ACD/BCF (pH 5. 5): | 244. 23 |
| ACD/KOC (pH 5. 5): | 1781. 51 |
| ACD/LogD (pH 7. 4): | 3. 44 |
| ACD/BCF (pH 7. 4): | 244. 23 |
| ACD/KOC (pH 7. 4): | 1781. 51 |
| Polar Surface Area: | 0 Å 2 |
| Polarizability: | 13. 9±0. 5 10 -24 cm 3 |
| Surface Tension: | 35. 4±3. 0 dyne/cm |
| Molar Volume: | 116. 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) = 3. 27Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 163. 30 (Adapted Stein & Brown method)Melting Pt (deg C): -40. 61 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 8 (Mean VP of Antoine & Grain methods)BP (exp database): 167 deg CVP (exp database): 2. 68E+00 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 88. 15log Kow used: 3. 27 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 155. 11 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Vinyl/Allyl HalidesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 27E-002 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 4. 832E-003 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 27 (KowWin est)Log Kaw used: -0. 285 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 3. 555Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 2164Biowin2 (Non-Linear Model) : 0. 0010Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 1090 (months )Biowin4 (Primary Survey Model) : 3. 1858 (weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 2308Biowin6 (MITI Non-Linear Model): 0. 0082Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 8034Ready 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): 357 Pa (2. 68 mm Hg)Log Koa (Koawin est ): 3. 555Kp (particle/gas partition coef. (m3/ug)): Mackay model : 8. 4E-009 Octanol/air (Koa) model: 8. 81E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 3. 03E-007 Mackay model : 6. 72E-007 Octanol/air (Koa) model: 7. 05E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 1. 1291 E-12 cm3/molecule-secHalf-Life = 9. 473 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 113. 672 HrsOzone Reaction: OVERALL Ozone Rate Constant = 0. 000461 E-17 cm3/molecule-secHalf-Life = 2488. 258 Days (at 7E11 mol/cm3)Fraction sorbed to airborne particulates (phi): 4. 87E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 206. 4Log Koc: 2. 315 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 = 1. 821 (BCF = 66. 27)log Kow used: 3. 27 (estimated)Volatilization from Water: Henry LC: 0. 0127 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 43 hoursHalf-Life from Model Lake : 128. 1 hours (5. 336 days)Removal In Wastewater Treatment: Total removal: 83. 84 percentTotal biodegradation: 0. 05 percentTotal sludge adsorption: 5. 09 percentTotal to Air: 78. 70 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 24. 5 226 1000 Water 32. 2 1. 44e+003 1000 Soil 41. 8 2. 88e+003 1000 Sediment 1. 55 1. 3e+004 0 Persistence Time: 265 hr

Click to predict properties on the Chemicalize site