1,1,2,3-tetrachloro-1-propene c3h2cl4 structure

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Molecular Formula	$C_3H_2Cl_4$
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)SynQuest63

457, 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

    sensitizerSynQuest1

    300-5-08, 63457

- Gas Chromatography

  - **Retention Index (Kovats):**

    1035 (estimated

    with error: 72)NIST

    Spectramainlib_115

    038

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

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