

# [Vinyl chloroacetate c4h5clo2 structure](https://assignbuster.com/vinyl-chloroacetate-c4h5clo2-structure/)

Contents

* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula  | C 4 H 5 ClO 2  |
| Average mass  | 120. 534 Da  |
| Density  | 1. 2±0. 1 g/cm 3  |
| Boiling Point  | 123. 7±23. 0 °C at 760 mmHg  |
| Flash Point  | 39. 0±18. 1 °C  |
| Molar Refractivity  | 26. 9±0. 3 cm 3  |
| Polarizability  | 10. 7±0. 5 10 -24 cm 3  |
| Surface Tension  | 29. 4±3. 0 dyne/cm  |
| Molar Volume  | 104. 5±3. 0 cm 3  |

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

## Experimental Boiling Point:

|  |
| --- |
| 136 °CAlfa Aesar  |
| 136 °CAlfa AesarL09446  |
| 37-38 °C / 16 mmHg (151. 5589-152. 8938 °C / 760 mmHg)LabNetworkLN00222863  |

## Experimental Flash Point:

|  |
| --- |
| 51 °CAlfa Aesar  |
| 51 °CAlfa Aesar  |
| 51 °F (10. 5556 °C)Alfa AesarL09446  |
| 51 °CLabNetworkLN00222863  |

## Experimental Gravity:

|  |
| --- |
| 1. 19 g/mLAlfa AesarL09446  |

## Experimental Refraction Index:

|  |
| --- |
| 1. 4435Alfa AesarL09446  |

* Miscellaneous

## Safety:

|  |
| --- |
| 10-23/24/25-34Alfa AesarL09446  |
| 26-36/37/39-45Alfa AesarL09446  |
| 6. 1Alfa AesarL09446  |
| CORROSIVEAlfa AesarL09446  |
| DangerAlfa AesarL09446  |
| DANGER: POISON, FLAMMABLE, causes CNS injuryAlfa AesarL09446  |
| H301-H311-H330-H314-H226Alfa AesarL09446  |
| P210-P301+P310-P303+P361+P353-P304+P340-P305+P351+P338-P320-P330-P361-P405-P501aAlfa AesarL09446  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 801 (estimated with error: 89)NIST Spectramainlib\_340488, replib\_229871, replib\_261933  |

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

|  |  |
| --- | --- |
| Density:  | 1. 2±0. 1 g/cm 3  |
| Boiling Point:  | 123. 7±23. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 13. 2±0. 2 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 36. 2±3. 0 kJ/mol  |
| Flash Point:  | 39. 0±18. 1 °C  |
| Index of Refraction:  | 1. 429  |
| Molar Refractivity:  | 26. 9±0. 3 cm 3  |
| #H bond acceptors:  | 2  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 3  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 0. 96  |
| ACD/LogD (pH 5. 5):  | 1. 06  |
| ACD/BCF (pH 5. 5):  | 3. 74  |
| ACD/KOC (pH 5. 5):  | 89. 46  |
| ACD/LogD (pH 7. 4):  | 1. 06  |
| ACD/BCF (pH 7. 4):  | 3. 74  |
| ACD/KOC (pH 7. 4):  | 89. 46  |
| Polar Surface Area:  | 26 Å 2  |
| Polarizability:  | 10. 7±0. 5 10 -24 cm 3  |
| Surface Tension:  | 29. 4±3. 0 dyne/cm  |
| Molar Volume:  | 104. 5±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. 98Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 139. 53 (Adapted Stein & Brown method)Melting Pt (deg C): -50. 01 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 6. 49 (Mean VP of Antoine & Grain methods)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1. 449e+004log Kow used: 0. 98 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 17313 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: EstersHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 4. 11E-004 atm-m3/moleGroup Method: 9. 09E-005 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 7. 104E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 98 (KowWin est)Log Kaw used: -1. 775 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 2. 755Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7530Biowin2 (Non-Linear Model) : 0. 9714Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 8998 (weeks )Biowin4 (Primary Survey Model) : 3. 8022 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 7664Biowin6 (MITI Non-Linear Model): 0. 7971Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 7987Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 796 Pa (5. 97 mm Hg)Log Koa (Koawin est ): 2. 755Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 77E-009 Octanol/air (Koa) model: 1. 4E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 36E-007 Mackay model : 3. 02E-007 Octanol/air (Koa) model: 1. 12E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 26. 4100 E-12 cm3/molecule-secHalf-Life = 0. 405 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 4. 860 HrsOzone Reaction: OVERALL Ozone Rate Constant = 0. 175000 E-17 cm3/molecule-secHalf-Life = 6. 549 Days (at 7E11 mol/cm3)Fraction sorbed to airborne particulates (phi): 2. 19E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 11. 85Log Koc: 1. 074 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 4. 150E+001 L/mol-secKb Half-Life at pH 8: 4. 639 hours Kb Half-Life at pH 7: 1. 933 days Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 0. 500 (BCF = 3. 162)log Kow used: 0. 98 (estimated)Volatilization from Water: Henry LC: 9. 09E-005 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 8. 192 hoursHalf-Life from Model Lake : 181. 4 hours (7. 559 days)Removal In Wastewater Treatment: Total removal: 6. 31 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 72 percentTotal to Air: 4. 49 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 2. 56 9. 15 1000 Water 46. 6 360 1000 Soil 50. 7 720 1000 Sediment 0. 093 3. 24e+003 0 Persistence Time: 247 hr

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