

# Vinyl chloroacetate $C_4H_5ClO_2$ structure

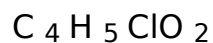


**ASSIGN  
BUSTER**

## Contents

- Retention Index (Kovats):

Molecular



Formula

Average mass 120. 534 Da

Density  $1.2 \pm 0.1 \text{ g/cm}^3$ Boiling Point  $123.7 \pm 23.0 \text{ }^\circ\text{C}$  at  
760 mmHgFlash Point  $39.0 \pm 18.1 \text{ }^\circ\text{C}$ 

Molar

$$26.9 \pm 0.3 \text{ cm}^3$$

Refractivity

Polarizability  $10.7 \pm 0.5 \cdot 10^{-24}$   
 $\text{cm}^3$ 

Surface

$$29.4 \pm 3.0 \text{ dyne/cm}$$

Tension

Molar Volume  $104.5 \pm 3.0 \text{ cm}^3$ 

- Experimental data
- Predicted - ACD/Labs
- Predicted - EPISuite

- Predicted - ChemAxon
- Experimental Physico-chemical Properties

- **Experimental Boiling Point:**

136 °C Alfa Aesar

136 °C Alfa

AesarL09446

37-38 °C / 16 mmHg

(151. 5589-152. 8938

°C / 760

mmHg) LabNetworkLN0

0222863

- **Experimental Flash Point:**

51 °C Alfa Aesar

51 °C Alfa Aesar

51 °F (10. 5556 °C) Alfa

AesarL09446

51 °C LabNetworkLN00222863

- **Experimental Gravity:**

1. 19 g/mL Alfa

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 <sup>3</sup>
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 <sup>3</sup>
#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 <sup>2</sup>

Polarizability:  $10.7 \pm 0.5 \times 10^{-24} \text{ cm}^3$

Surface Tension:  $29.4 \pm 3.0 \text{ dyne/cm}$

Molar Volume:  $104.5 \pm 3.0 \text{ cm}^3$

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. 98 Boiling 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+004 log Kow used: 0. 98 (estimated) no-melting pt equation used Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 17313 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Esters Henrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 4. 11E-004 atm-m<sup>3</sup>/mole Group Method: 9. 09E-005 atm-m<sup>3</sup>/mole Henrys LC [VP/WSol estimate using EPI values]: 7. 104E-005 atm-m<sup>3</sup>/mole Log 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. 755 Log Koa (experimental database): None Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7530 Biowin2 (Non-Linear Model) : 0. 9714 Expert 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. 7664 Biowin6 (MITI Non-Linear Model): 0. 7971 Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 7987 Ready Biodegradability Prediction: YES Hydrocarbon 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. 755 Kp (particle/gas partition coef. (m<sup>3</sup>/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 cm<sup>3</sup>/molecule-sec Half-Life = 0. 405 Days (12-hr day; 1. 5E6 OH/cm<sup>3</sup>) Half-Life = 4. 860 Hrs Ozone Reaction: OVERALL Ozone Rate Constant = 0. 175000 E-17 cm<sup>3</sup>/molecule-sec Half-Life = 6. 549 Days (at 7E11 mol/cm<sup>3</sup>) Fraction sorbed to airborne particulates (phi): 2. 19E-007 (Junge, Mackay) Note: the sorbed fraction may be resistant to atmospheric oxidation Soil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 11. 85 Log 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-sec Kb 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-m<sup>3</sup>/mole (estimated by Group SAR Method) Half-Life from Model River: 8. 192 hours Half-Life from Model Lake : 181. 4 hours (7. 559 days) Removal In Wastewater

Treatment: Total removal: 6.31 percent  
Total biodegradation: 0.09 percent  
Total sludge adsorption: 1.72 percent  
Total 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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