

# [Chloroacetone c3h5clo structure](https://assignbuster.com/chloroacetone-c3h5clo-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 3 H 5 ClO  |
| Average mass  | 92. 524 Da  |
| Density  | 1. 1±0. 1 g/cm 3  |
| Boiling Point  | 120. 0±8. 0 °C at 760 mmHg  |
| Flash Point  | 27. 8±0. 0 °C  |
| Molar Refractivity  | 20. 8±0. 3 cm 3  |
| Polarizability  | 8. 3±0. 5 10 -24 cm 3  |
| Surface Tension  | 25. 8±3. 0 dyne/cm  |
| Molar Volume  | 86. 6±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| -45 °CAlfa Aesar  |
| -44. 5 °COxford University Chemical Safety Data (No longer updated)More details  |
| -44. 5 °CJean-Claude Bradley Open Melting Point Dataset15014, 16696, 21172  |
| -45 °CJean-Claude Bradley Open Melting Point Dataset6620  |
| -45 °CAlfa AesarA11922  |
| -45 °CSynQuest2117-5-01  |
| -44. 5 °CBiosynthJ-504536  |

## Experimental Boiling Point:

|  |
| --- |
| 118-120 °CAlfa Aesar  |
| 120 °COxford University Chemical Safety Data (No longer updated)More details  |
| 118-120 °CAlfa AesarA11922  |
| 118-120 °CSynQuest2117-5-01  |
| 120 °CBiosynthJ-504536  |

## Experimental Flash Point:

|  |
| --- |
| 40 °CAlfa Aesar  |
| 27 °COxford University Chemical Safety Data (No longer updated)More details  |
| 40 °CSynQuest2117-5-01  |
| 40 °CAlfa Aesar  |
| 40 °F (4. 4444 °C)Alfa AesarA11922  |
| 35 °CSynQuest2117-5-01  |

## Experimental Gravity:

|  |
| --- |
| 20 g/mLMerck Millipore1374  |
| 20 g/lMerck Millipore1374, 802603  |
| 1. 161 g/mLSynQuest2117-5-01  |
| 25 g/mLSynQuest2117-5-01  |
| 1. 161 g/mLAlfa AesarA11922  |
| 1. 162 g/mLSynQuest2117-5-01  |
| 27. 8 g/mLBiosynthJ-504536  |

## Experimental Refraction Index:

|  |
| --- |
| 1. 434Alfa AesarA11922  |
| 1. 435SynQuest2117-5-01  |
| 1. 432SynQuest2117-5-01  |

* Miscellaneous

## Appearance:

|  |
| --- |
| colourless to dark yellow liquidOxford University Chemical Safety Data (No longer updated)More details  |

## Stability:

|  |
| --- |
| Stable. Incompatible with strong oxidizing agents, strong bases. May discolour on exposure to light. STENCH. Oxford University Chemical Safety Data (No longer updated)More details  |

## Toxicity:

|  |
| --- |
| ORL-RAT LD50 100 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

|  |
| --- |
| 10-23/24/25-34-50/53Alfa AesarA11922  |
| 26-36/37/39-45-60-61Alfa AesarA11922  |
| 6. 1Alfa AesarA11922  |
| DangerAlfa AesarA11922  |
| DANGER: FLAMMABLE, POISON, CORROSIVE, irritantAlfa AesarA11922  |
| DANGER: POISON, FLAMMABLE, causes CNS injuryAlfa AesarA11922  |
| H301-H310-H330-H314-H226-H400-H410Alfa AesarA11922  |
| Irritant/Flammable/Toxic/LachrymatorySynQuest2117-5-01  |
| P280-P273-P305+P351+P338-P309-P310-P501aAlfa AesarA11922  |
| R10, R24/25, R26, R36/37/38, R50/53SynQuest2117-5-01  |
| S9, S16, S23, S24/25, S26, S36/37/39, S45, S60, S61SynQuest2117-5-01  |
| Safety glasses, gloves, good ventilation. Oxford University Chemical Safety Data (No longer updated)More details  |
| Very Toxic/Flammable/Corrosive/Lachrymatory/Light Sensitive/Keep ColdSynQuest2117-5-01  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 681 (estimated with error: 89)NIST Spectramainlib\_19599, replib\_228991, replib\_154993, replib\_250272  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 675 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 20 mm; Column length: 25 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 50 C; End T: 250 C; CAS no: 78955; Active phase: OV-101; Carrier gas: N2/He; Phase thickness: 0. 10 um; Data type: Normal alkane RI; Authors: Zenkevich, I. G., Experimentally measured retention indices., 2005., Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 78955; Active phase: Polydimethyl siloxanes; Data type: Normal alkane RI; Authors: Zenkevich, I. G.; Chupalov, A. A., New Possibilities of Chromato Mass Pectrometric Identification of Organic Compounds Using Increments of Gas Chromatographic Retention Indices of Molecular Structural Fragments, Zh. Org. Khim. (Rus.), 32(5), 1996, 656-666, In original 656-666.)NIST Spectranist ri  |
| 653 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 0 C; End T: 250 C; CAS no: 78955; Active phase: DB-1; Data type: Normal alkane RI; Authors: Habu, T.; Flath, R. A.; Mon, T. R.; Morton, J. F., Volatile components of Rooibos tea (Aspalathus linearis), J. Agric. Food Chem., 33(2), 1985, 249-254.)NIST Spectranist ri  |
| 626. 4 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 2 mm; Column length: 50 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 20 C; End T: 200 C; Start time: 5 min; CAS no: 78955; Active phase: Methyl Silicone; Carrier gas: N2; Data type: Normal alkane RI; Authors: Yasuhara, A.; Morita, M.; Fuwa, K., Temperature-programmed retention indices of 221 halogenated organic compounds with 1-bromoalkanes as references, J. Chromatogr., 328, 1985, 35-48.)NIST Spectranist ri  |

## Retention Index (Linear):

|  |
| --- |
| 683 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 2. 5 K/min; Start T: 50 C; End T: 200 C; CAS no: 78955; Active phase: DB-5; Carrier gas: He; Phase thickness: 1 um; Data type: Linear RI; Authors: Dalluge, J.; van Stee, L. L. P.; Xu, X.; Williams, J.; Beens, J.; Vreuls, R. J. J.; Brinkman, U. A. Th., Unravelling the composition of very complex samples by comprehensive gas chromatography coupled to time-of-flight mass spectrometry. Cigarette smoke, J. Chromatogr. A, 974, 2002, 169-184.)NIST Spectranist ri  |

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

|  |  |
| --- | --- |
| Density:  | 1. 1±0. 1 g/cm 3  |
| Boiling Point:  | 120. 0±8. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 15. 5±0. 2 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 35. 8±3. 0 kJ/mol  |
| Flash Point:  | 27. 8±0. 0 °C  |
| Index of Refraction:  | 1. 397  |
| Molar Refractivity:  | 20. 8±0. 3 cm 3  |
| #H bond acceptors:  | 1  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 1  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 0. 43  |
| ACD/LogD (pH 5. 5):  | 0. 50  |
| ACD/BCF (pH 5. 5):  | 1. 40  |
| ACD/KOC (pH 5. 5):  | 44. 29  |
| ACD/LogD (pH 7. 4):  | 0. 50  |
| ACD/BCF (pH 7. 4):  | 1. 40  |
| ACD/KOC (pH 7. 4):  | 44. 29  |
| Polar Surface Area:  | 17 Å 2  |
| Polarizability:  | 8. 3±0. 5 10 -24 cm 3  |
| Surface Tension:  | 25. 8±3. 0 dyne/cm  |
| Molar Volume:  | 86. 6±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. 02Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 111. 24 (Adapted Stein & Brown method)Melting Pt (deg C): -59. 22 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 16. 4 (Mean VP of Antoine & Grain methods)MP (exp database): -44. 5 deg CBP (exp database): 119 deg CVP (exp database): 1. 20E+01 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1. 182e+005log Kow used: 0. 02 (estimated)no-melting pt equation usedWater Sol (Exper. database match) = 9e+004 mg/L (20 deg C)Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1. 3386e+005 mg/LWat Sol (Exper. database match) = 90000. 00Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 75E-005 atm-m3/moleGroup Method: 1. 20E-005 atm-m3/moleExper Database: 1. 65E-05 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 1. 689E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 02 (KowWin est)Log Kaw used: -3. 171 (exp database)Log Koa (KOAWIN v1. 10 estimate): 3. 191Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 5989Biowin2 (Non-Linear Model) : 0. 3518Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7990 (weeks )Biowin4 (Primary Survey Model) : 3. 5914 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6055Biowin6 (MITI Non-Linear Model): 0. 6219Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 3760Ready 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): 1. 6E+003 Pa (12 mm Hg)Log Koa (Koawin est ): 3. 191Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 87E-009 Octanol/air (Koa) model: 3. 81E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 6. 77E-008 Mackay model : 1. 5E-007 Octanol/air (Koa) model: 3. 05E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 3682 E-12 cm3/molecule-secHalf-Life = 29. 050 Days (12-hr day; 1. 5E6 OH/cm3)Ozone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 1. 09E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 3. 827Log Koc: 0. 583 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. 02 (estimated)Volatilization from Water: Henry LC: 1. 65E-005 atm-m3/mole (Henry experimental database)Half-Life from Model River: 35. 11 hours (1. 463 days)Half-Life from Model Lake : 463. 7 hours (19. 32 days)Removal In Wastewater Treatment: Total removal: 2. 75 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 74 percentTotal to Air: 0. 91 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 10. 3 697 1000 Water 44. 4 360 1000 Soil 45. 3 720 1000 Sediment 0. 082 3. 24e+003 0 Persistence Time: 349 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop