Chloroacetone c3h5clo structure

Contents

- Retention Index (Linear):

Molecular Formula	C_3H_5ClO
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-44. 5 °COxford University Chemical Safety Data (No longer updated)More details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 Oxford University Chemical Safety Data (No longer updated)More details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  ORL-RAT LD50 100 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details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/

LachrymatorySynQuest

2117-5-01

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/Corros

ive/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

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- 1-Click Docking
- 1-Click Scaffold Hop