# Glutaral c 5 h 8 o 2 structure

Contents

- Retention Index (Kovats):

| | |
|---|---|
| Molecular Formula | $C_5H_8O_2$ |
| Average mass | 100. 116 Da |
| Density | $0.9 \pm 0.1$ g/cm $^3$ |
| Boiling Point | 189. 0±13. 0 °C at 760 mmHg |
| Flash Point | 66. 0±16. 8 °C |
| Molar Refractivity | 25. 6±0. 3 cm $^3$ |
| Polarizability | $10.1 \pm 0.5 \times 10^{-24}$ cm $^3$ |
| Surface Tension | 30. 7±3. 0 dyne/cm |
| Molar Volume | 105. 7±3. 0 cm $^3$ |

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite
- Predicted – ChemAxon
- Predicted – Mcule

- Experimental Physico-chemical Properties

  - **Experimental Melting Point:**

    -21 °CAlfa Aesar

    -6 °COxford University Chemical Safety Data (No longer updated)More details

    -6 °CJean-Claude Bradley Open Melting Point Dataset15816

    -21 °CJean-Claude Bradley Open Melting Point Dataset7260

    -21 °CAlfa AesarA10500

    -21 °CSynQuest75281, 2115-1-07

    -15 °CBiosynthQ-201162

    -15 °CLabNetworkLN00220666

    -14 °CFooDBFDB000763

  - **Experimental Boiling Point:**

    100 °CAlfa Aesar

    212 F (100 °C)NIOSHMA2450000

    101 °COxford University Chemical Safety Data (No longer updated)More details

    100 °CAlfa AesarA10500

101 °CSynQuest75281, 2115-1-07

189 °CBiosynthQ-201162

100 °CLabNetworkLN00220666

10 °C / 71 mmHg (75. 4546 °C / 760 mmHg)FooDBFDB000763

- **Experimental Vapor Pressure:**

  17

  mmHgNIOSHMA2450000

- **Experimental Flash Point:**

  66 °CBiosynthQ-201162

  100

  °CLabNetworkLN00220666

- **Experimental Freezing Point:**

  7 F (-13. 8889

  °C)NIOSHMA2450000

- **Experimental Gravity:**

  0. 947 g/mLBiosynthQ-

  201162

25 g/mLSynQuest2115-1-

07

1. 123 g/mLAlfa

AesarA10500

1. 062 g/mLAlfa

AesarA17876

1. 106 g/mLSynQuest2115-

1-07

66 g/mLBiosynthQ-201162

1. 12-1. 14

g/lFluorochem358208

- **Experimental Refraction Index:**

  1. 373Alfa

  AesarA17876

  20FooDBFDB000763

- **Experimental Solubility:**

  MiscibleNIOSHMA24500

  00

- Miscellaneous

- **Appearance:**

  Colorless liquid with a pungent odor. NIOSHMA2450000

  colourless or light yellow liquid with a pungent odourOxford University Ch

  Safety Data (No longer updated)More details

- **Stability:**

  Stable. Incompatible with strong bases, strong acids, strong oxidizing ag

  May discolour upon exposure to air. Keep cold. Oxford University Chemic

  Data (No longer updated)More details

- **Toxicity:**

  ORL-RAT LD50 134 mg kg-1 , SKN-RBT LD50 > 2500 mg kg-1 , IPR-RAT L

  9 mg kg-1 , ORL-GPG LD50 50 mg kg-1Oxford University Chemical Safety

  (No longer updated)More details

- **Safety:**

  22-23-34-37-42/43Alfa AesarA17876

  23/25-34-37-42/43-50Alfa AesarA10500

  26-36/37/39-45-60-61Alfa AesarA17876

  4-9-20-23-26-36/37/39-45-57Alfa AesarA10500

  8Alfa AesarA10500, A17876

  DangerAlfa AesarA10500, A17876

DangerBiosynthQ-201162

DANGER: CORROSIVE, burns skin and eyesAlfa AesarA17876

DANGER: CORROSIVE, POISON, burns skin and eyesAlfa AesarA10500, A1

DANGER: POISON, CORROSIVE, irritates eyes, skin, lungsAlfa AesarA1050

GHS05; GHS07; GHS08; GHS09BiosynthQ-201162

H301-H331-H334-H314-H400-H317-H335-H336Alfa AesarA10500

H302; H314; H317; H332; H334; H370; H400BiosynthQ-201162

H331-H334-H314-H400-H302-H317-H335-H336Alfa AesarA17876

keep cold/Corrosive/Toxic/very toxic to aquatic lifeSynQuest2115-1-07, 7

P260; P273; P280; P305+P351+P338; P310BiosynthQ-201162

P260-P285-P303+P361+P353-P305+P351+P338-P405-P501aAlfa AesarA

P260-P301+P310-P303+P361+P353-P305+P351+P338-P405-P501aAlfa AesarA10500

R25, R26, R34, R41, R42, R43, R50SynQuest2115-1-07, 75281

S13, S23, S24/25, S26, S28, S36/37/39, S45SynQuest2115-1-07, 75281

Safety glasses, gloves, good ventilation. Oxford University Chemical Safe

(No longer updated)More details

- **First-Aid:**

  Eye: Irrigate immediately Skin: Water flush immediately Breathing: Resp

  support Swallow: Medical attention immediatelyNIOSHMA2450000

- **Exposure Routes:**

  inhalation, skin absorption, ingestion, skin and/or eye

  contactNIOSHMA2450000

- **Symptoms:**

  Irritation eyes, skin, respiratory system; dermatitis, sensitization skin; co

  asthma; nausea, vomitingNIOSHMA2450000

- **Target Organs:**

  Eyes, skin, respiratory

  systemNIOSHMA2450000

- **Incompatibility:**

  Strong oxidizers, strong bases [Note: Alkaline solutions of glutaraldehyde

  activated glutaraldehyde) react with alcohol, ketones, amines, hydrazine

  proteins.]NIOSHMA2450000

- **Personal Protection:**

  Skin: Prevent skin contact Eyes: Prevent eye contact Wash skin: When

  contaminated Remove: When wet or contaminated Change: No recomme

Provide: Eyewash, Quick drenchNIOSHMA2450000

- **Exposure Limits:**

  NIOSH REL : C 0. 2 ppm (0. 8 mg/m 3 ) See Appendix C (Aldehydes) OSH

  noneNIOSHMA2450000

- Gas Chromatography

- **Retention Index (Kovats):**

  895 (estimated with error: 45)NIST

  Spectramainlib_341303, replib_1116

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

| | |
|---|---|
| Density: | 0. 9±0. 1 g/cm $^3$ |
| Boiling Point: | 189. 0±13. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 6±0. 4 mmHg at 25°C |
| Enthalpy of Vaporization: | 42. 5±3. 0 kJ/mol |
| Flash Point: | 66. 0±16. 8 °C |
| Index of Refraction: | 1. 399 |
| Molar Refractivity: | 25. 6±0. 3 cm $^3$ |
| #H bond acceptors: | 2 |

| | |
|---|---|
| #H bond donors: | 0 |
| #Freely Rotating Bonds: | 4 |
| #Rule of 5 Violations: | 0 |
| ACD/LogP: | -0. 34 |
| ACD/LogD (pH 5. 5): | 0. 18 |
| ACD/BCF (pH 5. 5): | 1. 00 |
| ACD/KOC (pH 5. 5): | 29. 90 |
| ACD/LogD (pH 7. 4): | 0. 18 |
| ACD/BCF (pH 7. 4): | 1. 00 |
| ACD/KOC (pH 7. 4): | 29. 90 |
| Polar Surface Area: | 34 Å $^{2}$ |
| Polarizability: | 10. 1±0. 5 10 $^{-24}$ cm $^{3}$ |
| Surface Tension: | 30. 7±3. 0 dyne/cm |
| Molar Volume: | 105. 7±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. 18Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 166. 10 (Adapted Stein & Brown method)Melting Pt (deg C): -29. 86 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 88 (Mean VP of Antoine & Grain methods)BP (exp database): 188 dec deg CVP (exp database): 6. 00E-01 mm Hg at 30 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1. 672e+005log Kow used: -0. 18 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 7. 0998e+005 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: AldehydesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 10E-007 atm-m3/moleGroup Method: 2. 39E-008 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 1. 481E-006 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -0. 18 (KowWin est)Log Kaw used: -5. 347 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 5. 167Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 1. 2691Biowin2 (Non-Linear Model) : 1. 0000Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 0226 (weeks )Biowin4 (Primary Survey Model) : 4. 0966 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 1. 3853Biowin6 (MITI Non-Linear Model): 0. 9984Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 1. 1592Ready 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): 80 Pa (0. 6 mm Hg)Log Koa (Koawin est ): 5. 167Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 75E-008 Octanol/air (Koa) model: 3. 61E-008 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 35E-006 Mackay model : 3E-006 Octanol/air (Koa) model: 2. 88E-006 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 46. 8857 E-12 cm3/molecule-secHalf-Life = 0. 228 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 2. 738 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 18E-006 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 094Log Koc: 0. 039 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. 18 (estimated)Volatilization from Water: Henry LC: 2. 39E-008 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 2. 451E+004 hours (1021 days)Half-Life from Model Lake : 2. 675E+005 hours (1. 115E+004 days)Removal In Wastewater Treatment: Total removal: 1. 85 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 76 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 4 10. 8 1000 Water 41. 2 360 1000 Soil 58. 3 720 1000 Sediment 0. 0759 3. 24e+003 0 Persistence Time: 484 hr