Ethyl acetopyruvate c7h10o4 structure

Contents

- Retention Index (Kovats):

Molecular Formula	$C_7H_{10}O_4$
Average mass	158. 152 Da
Density	1. 1±0. 1 g/cm ^{3}
Boiling Point	214. 7±13. 0 °C at 760 mmHg
Flash Point	85. 8±19. 9 °C
Molar Refractivity	36. 3±0. 3 cm ^{3}
Polarizability	14. 4±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	35. 2±3. 0 dyne/cm
Molar Volume	141. 8±3. 0 cm ^{3}

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

- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties

Experimental Melting Point:

16-18 °CAlfa Aesar

18 °CJean-Claude

Bradley Open Melting

Point Dataset23380

16-18 °CMatrix

Scientific

16-18 °CAlfa

AesarA13808

16-18 °CMatrix

Scientific059041

18

°CAcemolAMOT0290

16-18

°CLabNetworkLN00009

536

- **Experimental Boiling Point:**

  108-109 deg C / 12 mm

  (256. 1568-257. 51 °C /

  760 mmHg)Alfa Aesar

  108-109 ° / 12 mm

  (256. 1568-257. 51 °C /

  760 mmHg)Matrix

  Scientific

  108-109 °C / 12 mm

  (256. 1568-257. 51 °C /

  760 mmHg)Alfa

  AesarA13808

  108-109 °C / 12 mm

  (256. 1568-257. 51 °C /

  760 mmHg)Matrix

  Scientific059041

  86. 5 °C / 5 Torr (255.

  8103 °C / 760

  mmHg)AcemolAMOT02

  90

  108-109 °C / 12 mm

  (256. 1568-257. 51 °C /

  760

mmHg)LabNetworkLN0

0009536

- **Experimental Flash Point:**

  110 °CAlfa Aesar

  110 °CAlfa Aesar

  110 °F (43. 3333 °C)Alfa

  AesarA13808

  113 °CAcemolAMOT0290

  230 °CLabNetworkLN00009536

- **Experimental Gravity:**

  1. 126 g/mLAlfa AesarA13808

  1. 126 g/mLMatrix

  Scientific059041

  1. 126

  g/mLAcemolAMOT0290

  1. 126 g/mLFluorochem

  1. 126 g/lFluorochem067147

- **Experimental Refraction Index:**

  1. 473Alfa

  AesarA13808

- Miscellaneous

- **Appearance:**

  Not AvailableNovochemy[NC-

  14185]

- **Safety:**

  20/21/22Novochemy[N

  C-14185]

  20/21/36/37/39Novoch

  emy[NC-14185]

  CAUTION: May irritate

  eyes, respiratory

  tractAlfa AesarA13808

  GHS07;

  GHS09Novochemy[NC-

  14185]

  H332;

  H403Novochemy[NC-

14185]

IRRITANTMatrix Scientific059041

Irritant/Keep ColdSynQuest2129-1-30

P332+P313; P305+P351+P338Novochemy[NC-14185]

WarningNovochemy[NC-14185]

XnNovochemy[NC-14185]

- Gas Chromatography

  - **Retention Index (Kovats):**
    1156 (estimated with error: 89)NIST Spectramainlib_342255, replib_239629

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

Density:	1. 1±0. 1 g/cm ^{3}
Boiling Point:	214. 7±13. 0 °C at 760 mmHg
Vapour Pressure:	0. 2±0. 4 mmHg at 25°C
Enthalpy of Vaporization:	45. 1±3. 0 kJ/mol
Flash Point:	85. 8±19. 9 °C
Index of Refraction:	1. 426
Molar Refractivity:	36. 3±0. 3 cm ^{3}
#H bond acceptors:	4
#H bond donors:	0
#Freely Rotating Bonds:	5
#Rule of 5 Violations:	0
ACD/LogP:	-0. 19
ACD/LogD (pH 5. 5):	-0. 04
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	22. 36
ACD/LogD (pH 7. 4):	-0. 66

ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	5. 32
Polar Surface Area:	60 Å ^{2}
Polarizability:	14. 4±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	35. 2±3. 0 dyne/cm
Molar Volume:	141. 8±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) = -1. 53Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 227. 94 (Adapted Stein & Brown method)Melting Pt (deg C): 28. 56 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 178 (Mean VP of Antoine & Grain methods)MP (exp database): 18 deg CBP (exp database): 214 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1e+006log Kow used: -1. 53 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 3. 8342e+005 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: EstersHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 6. 23E-010 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 3. 704E-008 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -1. 53 (KowWin est)Log Kaw used: -7. 594 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 6. 064Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8533Biowin2 (Non-Linear Model) : 0. 9877Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 9674 (weeks)Biowin4 (Primary Survey Model) : 3. 8263 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 8028Biowin6 (MITI Non-Linear Model): 0. 8945Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 5089Ready 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): 22 Pa (0. 165 mm Hg)Log Koa (Koawin est): 6. 064Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 36E-007 Octanol/air (Koa) model: 2. 84E-007 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 4. 93E-006 Mackay model : 1. 09E-005 Octanol/air

(Koa) model: 2. 28E-005 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 2. 2891 E-12 cm3/molecule-secHalf-Life = 4. 673 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 56. 072 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 7. 92E-006 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 10Log Koc: 1. 000 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: -1. 53 (estimated)Volatilization from Water: Henry LC: 6. 23E-010 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 182E+006 hours (4. 925E+004 days)Half-Life from Model Lake : 1. 289E+007 hours (5. 372E+005 days)Removal In Wastewater Treatment: Total removal: 1. 85 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 75 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. 0147 112 1000 Water 39 360 1000 Soil 60. 9 720 1000 Sediment 0. 0714 3. 24e+003 0 Persistence Time: 578 hr

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