

# [Ethyl acetopyruvate c7h10o4 structure](https://assignbuster.com/ethyl-acetopyruvate-c7h10o4-structure/)

Contents

* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula  | C 7 H 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 °CLabNetworkLN00009536  |

## 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)AcemolAMOT0290  |
| 108-109 °C / 12 mm (256. 1568-257. 51 °C / 760 mmHg)LabNetworkLN00009536  |

## 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[NC-14185]  |
| 20/21/36/37/39Novochemy[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

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop