

# [2-acetoxy-3-butanone c6h10o3 structure](https://assignbuster.com/2-acetoxy-3-butanone-c6h10o3-structure/)

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* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula | C 6 H 10 O 3 |
| Average mass | 130. 142 Da |
| Density | 1. 0±0. 1 g/cm 3 |
| Boiling Point | 163. 4±23. 0 °C at 760 mmHg |
| Flash Point | 56. 6±22. 7 °C |
| Molar Refractivity | 31. 6±0. 3 cm 3 |
| Polarizability | 12. 5±0. 5 10 -24 cm 3 |
| Surface Tension | 28. 9±3. 0 dyne/cm |
| Molar Volume | 128. 6±3. 0 cm 3 |

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

## Experimental Boiling Point:

|  |
| --- |
| 154-155 °CAlfa Aesar |
| 74-75 °C / 20 mm Hg (193. 7316-195. 0446 °C / 760 mmHg)Food and Agriculture Organization of the United Nations1-Methyl-2-oxopropyl acetate |
| 154-155 °CAlfa AesarL06927 |
| 169-173 °CFooDBFDB011808 |

## Experimental Flash Point:

|  |
| --- |
| 66 °CAlfa Aesar |
| 66 °CAlfa Aesar |
| 66 °F (18. 8889 °C)Alfa AesarL06927 |

## Experimental Gravity:

|  |
| --- |
| 1. 025 g/mLAlfa AesarL06927 |

## Experimental Refraction Index:

|  |
| --- |
| 1. 412Alfa AesarL06927 |
| 1. 41-1. 416Food and Agriculture Organization of the United Nations1-Methyl-2-oxopropyl acetate |

* Miscellaneous

## Appearance:

|  |
| --- |
| colourless to slightly yellow liquidFood and Agriculture Organization of the United Nations1-Methyl-2-oxopropyl acetate |

## Safety:

|  |
| --- |
| 23-26-37Alfa AesarL06927 |
| 36/38Alfa AesarL06927 |
| H315-H319Alfa AesarL06927 |
| IRRITANTAlfa AesarL06927 |
| P280-P305+P351+P338-P362-P321-P332+P313-P337+P313Alfa AesarL06927 |
| WarningAlfa AesarL06927 |
| WARNING: Irritates skin and eyesAlfa AesarL06927 |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 857 (estimated with error: 89)NIST Spectramainlib\_352267 |

## Retention Index (Normal Alkane):

|  |
| --- |
| 857 (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: 5 K/min; Start T: 65 C; End T: 280 C; End time: 30 min; Start time: 10 min; CAS no: 4906245; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickness: 0. 4 um; Data type: Normal alkane RI; Authors: Joulain, D.; Casazza, A.; Laurent, R.; Portier, D.; Guillamon, N.; Pandya, R.; Le, M.; Viljoen, A., Volatile flavor constituents of fruits from Southern Africa: mobola plum (Parinari curatellifolia), J. Agric. Food Chem., 52, 2004, 2322-2325.)NIST Spectranist ri |
| 852 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 50 C; End T: 240 C; Start time: 3 min; CAS no: 4906245; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Shiota, H., New esteric components in the volatiles of banana fruit (Musa sapientum L.), J. Agric. Food Chem., 41(11), 1993, 2056-2062.)NIST Spectranist ri |
| 856 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 50 C; End T: 240 C; Start time: 3 min; CAS no: 4906245; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Shiota, H., New esteric components in the volatiles of banana fruit (Musa sapientum L.), J. Agric. Food Chem., 41(11), 1993, 2056-2062., Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 50 C; End T: 240 C; CAS no: 4906245; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Shiota, H., Volatile components of pawpaw fruit (Asimina triloba Dunal.), J. Agric. Food Chem., 39(9), 1991, 1631-1635.)NIST Spectranist ri |
| 855 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 50 C; End T: 240 C; CAS no: 4906245; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Shiota, H., Volatile components of pawpaw fruit (Asimina triloba Dunal.), J. Agric. Food Chem., 39(9), 1991, 1631-1635.)NIST Spectranist ri |
| 1378 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 40 C; End T: 220 C; End time: 10 min; Start time: 10 min; CAS no: 4906245; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Hayata, Y.; Sakamoto, T.; Kozuka, H.; Sakamoto, K.; Osajima, Y., Analysis of aromatic volatile compounds in ‘ Miyabi’ melon (Cucumis melo L.) using the Porapak Q column, J. Jpn. Soc. Hortic. Sci., 71(4), 2002, 517-525.)NIST Spectranist ri |

## Retention Index (Linear):

|  |
| --- |
| 1389 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 40 C; End T: 250 C; End time: 15 min; Start time: 3 min; CAS no: 4906245; Active phase: DB-Wax Etr; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Aubert C.; Pitrat M., Volatile compounds in the skin and pulp of Queen Anne’s pocket melon, J. Agric. Food Chem., 54, 2006, 8177-8182., Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 40 C; End T: 240 C; Start time: 2 min; CAS no: 4906245; Active phase: DB-FFAP; Carrier gas: H2; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Charles, M.; Martin, B.; Ginies, C.; Etievant, P.; Coste, G.; Guichard, E., Potent aroma compounds of two red wine vinegars, J. Agric. Food Chem., 48, 2000, 70-77.)NIST Spectranist ri |
| 1377 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 40 C; End T: 200 C; Start time: 10 min; CAS no: 4906245; Active phase: DB-Wax; Carrier gas: He; Data type: Linear RI; Authors: Umano, K.; Hagi, Y.; Nakahara, K.; Shoji, A.; Shibamoto, T., Volatile constituents of green and ripened pineapple (Aanas comosus [L.] Merr.), J. Agric. Food Chem., 40(4), 1992, 599-603.)NIST Spectranist ri |
| 1358 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 50 C; End T: 250 C; Start time: 3 min; CAS no: 4906245; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Frohlich, O.; Duque, C.; Schreier, P., Volatile constituents of curuba (Passiflora mollissima) fruit, J. Agric. Food Chem., 37(2), 1989, 421-425.)NIST Spectranist ri |
| 1361 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 50 C; End T: 250 C; Start time: 3 min; CAS no: 4906245; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Frohlich, O.; Duque, C.; Schreier, P., Volatile constituents of curuba (Passiflora mollissima) fruit, J. Agric. Food Chem., 37(2), 1989, 421-425.)NIST Spectranist ri |

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

|  |  |
| --- | --- |
| Density: | 1. 0±0. 1 g/cm 3 |
| Boiling Point: | 163. 4±23. 0 °C at 760 mmHg |
| Vapour Pressure: | 2. 1±0. 3 mmHg at 25°C |
| Enthalpy of Vaporization: | 40. 0±3. 0 kJ/mol |
| Flash Point: | 56. 6±22. 7 °C |
| Index of Refraction: | 1. 406 |
| Molar Refractivity: | 31. 6±0. 3 cm 3 |
| #H bond acceptors: | 3 |
| #H bond donors: | 0 |
| #Freely Rotating Bonds: | 3 |
| #Rule of 5 Violations: | 0 |

|  |  |
| --- | --- |
| ACD/LogP: | 0. 68 |
| ACD/LogD (pH 5. 5): | 0. 26 |
| ACD/BCF (pH 5. 5): | 1. 00 |
| ACD/KOC (pH 5. 5): | 33. 10 |
| ACD/LogD (pH 7. 4): | 0. 26 |
| ACD/BCF (pH 7. 4): | 1. 00 |
| ACD/KOC (pH 7. 4): | 33. 10 |
| Polar Surface Area: | 43 Å 2 |
| Polarizability: | 12. 5±0. 5 10 -24 cm 3 |
| Surface Tension: | 28. 9±3. 0 dyne/cm |
| Molar Volume: | 128. 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. 22Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 156. 08 (Adapted Stein & Brown method)Melting Pt (deg C): -30. 52 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 3. 02 (Mean VP of Antoine & Grain methods)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 5. 921e+004log Kow used: 0. 22 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 3. 1895e+005 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: EstersHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 11E-006 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 8. 734E-006 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 22 (KowWin est)Log Kaw used: -4. 343 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 4. 563Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8666Biowin2 (Non-Linear Model) : 0. 9917Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 0293 (weeks )Biowin4 (Primary Survey Model) : 3. 8667 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 7370Biowin6 (MITI Non-Linear Model): 0. 8815Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 2115Ready 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): 367 Pa (2. 75 mm Hg)Log Koa (Koawin est ): 4. 563Kp (particle/gas partition coef. (m3/ug)): Mackay model : 8. 18E-009 Octanol/air (Koa) model: 8. 97E-009 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 2. 96E-007 Mackay model : 6. 55E-007 Octanol/air (Koa) model: 7. 18E-007 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 3. 0026 E-12 cm3/molecule-secHalf-Life = 3. 562 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 42. 747 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 4. 75E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 634Log Koc: 0. 213 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 9. 082E-002 L/mol-secKb Half-Life at pH 8: 88. 325 days Kb Half-Life at pH 7: 2. 418 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 0. 500 (BCF = 3. 162)log Kow used: 0. 22 (estimated)Volatilization from Water: Henry LC: 1. 11E-006 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 602. 9 hours (25. 12 days)Half-Life from Model Lake : 6673 hours (278 days)Removal In Wastewater Treatment: Total removal: 1. 92 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 76 percentTotal to Air: 0. 06 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 4. 58 85. 5 1000 Water 44. 5 360 1000 Soil 50. 8 720 1000 Sediment 0. 0828 3. 24e+003 0 Persistence Time: 382 hr

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