

# [Acetaldehyde ammonia trimer c6h15n3 structure](https://assignbuster.com/acetaldehyde-ammonia-trimer-c6h15n3-structure/)

Contents

* Safety:

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| --- | --- |
| Molecular Formula | C 6 H 15 N 3 |
| Average mass | 129. 203 Da |
| Density | 0. 8±0. 1 g/cm 3 |
| Boiling Point | 110. 0±0. 0 °C at 760 mmHg |
| Flash Point | 15. 4±13. 5 °C |
| Molar Refractivity | 38. 0±0. 3 cm 3 |
| Polarizability | 15. 1±0. 5 10 -24 cm 3 |
| Surface Tension | 22. 5±3. 0 dyne/cm |
| Molar Volume | 154. 5±3. 0 cm 3 |

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

## Experimental Melting Point:

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| --- |
| 93-96 °CAlfa Aesar |
| 93-96 °CAlfa AesarL12265 |

## Experimental Boiling Point:

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| 110 °C (Decomposes)Alfa Aesar |
| 110 °C (Decomposes)Alfa AesarL12265 |

## Experimental Gravity:

|  |
| --- |
| 0. 852 g/mLAlfa AesarL12265 |

* Miscellaneous

## Safety:

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| 26-37Alfa AesarL12265 |
| 36/37/38Alfa AesarL12265 |
| DANGER: FLAMMABLE, irritates skin, eyes, lungsAlfa AesarL12265 |

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

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| --- | --- |
| Density: | 0. 8±0. 1 g/cm 3 |
| Boiling Point: | 110. 0±0. 0 °C at 760 mmHg |
| Vapour Pressure: | 24. 2±0. 2 mmHg at 25°C |
| Enthalpy of Vaporization: | 34. 9±3. 0 kJ/mol |
| Flash Point: | 15. 4±13. 5 °C |
| Index of Refraction: | 1. 407 |
| Molar Refractivity: | 38. 0±0. 3 cm 3 |
| #H bond acceptors: | 3 |
| #H bond donors: | 3 |
| #Freely Rotating Bonds: | 0 |
| #Rule of 5 Violations: | 0 |

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| --- | --- |
| ACD/LogP: | 0. 43 |
| ACD/LogD (pH 5. 5): | -2. 82 |
| ACD/BCF (pH 5. 5): | 1. 00 |
| ACD/KOC (pH 5. 5): | 1. 00 |
| ACD/LogD (pH 7. 4): | -1. 56 |
| ACD/BCF (pH 7. 4): | 1. 00 |
| ACD/KOC (pH 7. 4): | 1. 00 |
| Polar Surface Area: | 36 Å 2 |
| Polarizability: | 15. 1±0. 5 10 -24 cm 3 |
| Surface Tension: | 22. 5±3. 0 dyne/cm |
| Molar Volume: | 154. 5±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): 237. 87 (Adapted Stein & Brown method)Melting Pt (deg C): 68. 48 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0193 (Modified Grain method)Subcooled liquid VP: 0. 0495 mm Hg (25 deg C, Mod-Grain method)Water 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) = 1e+006 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 09E-005 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 3. 281E-009 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -1. 53 (KowWin est)Log Kaw used: -3. 068 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 1. 538Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 1. 1475Biowin2 (Non-Linear Model) : 0. 9891Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 9870 (weeks )Biowin4 (Primary Survey Model) : 3. 7912 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4662Biowin6 (MITI Non-Linear Model): 0. 0841Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 1. 2476Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 6. 6 Pa (0. 0495 mm Hg)Log Koa (Koawin est ): 1. 538Kp (particle/gas partition coef. (m3/ug)): Mackay model : 4. 55E-007 Octanol/air (Koa) model: 8. 47E-012 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 64E-005 Mackay model : 3. 64E-005 Octanol/air (Koa) model: 6. 78E-010 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 692. 8737 E-12 cm3/molecule-secHalf-Life = 0. 015 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 11. 115 MinOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 64E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 126. 4Log Koc: 2. 102 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: 2. 09E-005 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 33 hours (1. 375 days)Half-Life from Model Lake : 455. 3 hours (18. 97 days)Removal In Wastewater Treatment: Total removal: 2. 97 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 74 percentTotal to Air: 1. 15 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 0771 0. 371 1000 Water 49. 5 360 1000 Soil 50. 3 720 1000 Sediment 0. 0906 3. 24e+003 0 Persistence Time: 296 hr

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