# Acetic acid, cyclohexyl ester

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|---|---|
| **Other names:** | Acetoxycyclohexane |
| | Cyclohexanol, acetate |
| | Cyclohexanolazetat |
| | Cyclohexanyl acetate |
| | Cyclohexyl acetate |
| | Cyclohexyl ester of acetic acid |
| | Cyclohexylester kyseliny octove |
| | Hexalin acetate |
| | NSC 8772 |
| | UN 2243 |
| | cyclohexanol acetate |
| | cyclohexyl ethanoate |
| | ethanoic acid, cyclohexyl ester |
| **Inchi:** | InChI=1S/C8H14O2/c1-7(9)10-8-5-3-2-4-6-8/h8H,2-6H2,1H3 |
| **InchiKey:** | YYLLIJHXUHJATK-UHFFFAOYSA-N |
| **Formula:** | C8H14O2 |
| **SMILES:** | CC(=O)OC1CCCCC1 |
| **Mol. weight [g/mol]:** | 142.20 |
| **CAS:** | 622-45-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -4590.00 ± 2.80 | kJ/mol | NIST Webbook |
| gf | -192.99 | kJ/mol | Joback Method |
| hf | -507.20 ± 3.00 | kJ/mol | NIST Webbook |
| hfl | -558.90 ± 3.00 | kJ/mol | NIST Webbook |
| hfus | 11.10 | kJ/mol | Joback Method |
| hvap | 42.99 | kJ/mol | Joback Method |
| log10ws | -1.67 | | Aqueous Solubility Prediction Method |
| logp | 1.882 | | Crippen Method |
| mcvol | 120.160 | ml/mol | McGowan Method |
| pc | 3322.01 | kPa | Joback Method |
| rinpol | 1043.00 | | NIST Webbook |
| rinpol | 1043.00 | | NIST Webbook |
| rinpol | 1043.00 | | NIST Webbook |
| rinpol | 1043.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1043.00 | | NIST Webbook |
| rinpol | 1017.00 | | NIST Webbook |
| rinpol | 1024.00 | | NIST Webbook |
| rinpol | 1042.00 | | NIST Webbook |
| rinpol | 1027.00 | | NIST Webbook |
| rinpol | 1024.00 | | NIST Webbook |
| rinpol | 1027.00 | | NIST Webbook |
| rinpol | 1024.00 | | NIST Webbook |
| rinpol | 1010.00 | | NIST Webbook |
| rinpol | 1023.00 | | NIST Webbook |
| rinpol | 999.00 | | NIST Webbook |
| rinpol | 1043.00 | | NIST Webbook |
| rinpol | 1010.00 | | NIST Webbook |
| rinpol | 1043.00 | | NIST Webbook |
| rinpol | 1043.00 | | NIST Webbook |
| ripol | 1343.00 | | NIST Webbook |
| ripol | 1379.00 | | NIST Webbook |
| tb | 447.00 | K | NIST Webbook |
| tb | 450.20 ± 1.00 | K | NIST Webbook |
| tb | 446.26 ± 0.20 | K | NIST Webbook |
| tb | 446.20 | K | NIST Webbook |
| tc | 689.84 | K | Joback Method |
| tf | 259.46 | K | Joback Method |
| tt | 224.64 ± 0.15 | K | NIST Webbook |
| vc | 0.441 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 336.02 | J/mol×K | 654.58 | Joback Method |
| cpg | 263.26 | J/mol×K | 478.28 | Joback Method |
| cpg | 279.37 | J/mol×K | 513.54 | Joback Method |
| cpg | 294.69 | J/mol×K | 548.80 | Joback Method |
| cpg | 309.24 | J/mol×K | 584.06 | Joback Method |
| cpg | 323.01 | J/mol×K | 619.32 | Joback Method |
| cpg | 348.27 | J/mol×K | 689.84 | Joback Method |

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|---|---|---|---|---|---|
| dvisc | 0.0010100 | Pa×s | 340.00 | Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material) | |
| dvisc | 0.0011600 | Pa×s | 330.00 | Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material) | |
| dvisc | 0.0013600 | Pa×s | 320.00 | Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material) | |
| dvisc | 0.0016100 | Pa×s | 310.00 | Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material) | |
| dvisc | 0.0019500 | Pa×s | 300.00 | Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material) | |
| hfust | 8.00 | kJ/mol | 224.60 | NIST Webbook | |
| hvapt | 52.16 | kJ/mol | 300.11 | Comprehensive Study of Vapor Pressures and Enthalpies of Vaporization of Cyclohexyl Esters | |
| hvapt | 46.70 | kJ/mol | 407.00 | NIST Webbook | |
| rfi | 1.44100 | | 293.20 | Phase Equilibria for the Ternary Liquid Systems of (Water + Tetrahydrofurfuryl Alcohol + Cyclic Solvent) at 298.2 K | |

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|---|---|---|---|
| rfi | 1.44250 | 293.15 | Liquid-liquid equilibria study of the (water + phosphoric acid + hexyl or cyclohexyl acetate) systems at T = (298.15, 308.15, and 318.15) K: Measurement and thermodynamic modelling |
| rfi | 1.44340 | 293.15 | (Liquid + liquid) equilibria of (water + butyric acid + cyclohexyl acetate) ternary system |
| rfi | 1.44220 | 293.15 | Phase equilibria of water + 1-propanol + solvent (n-amyl acetate, cyclohexanol, and cyclohexyl acetate) at T = 298.2K |
| rfi | 1.43980 | 293.00 | Quaternary Liquid-Liquid Equilibrium of Water + Acetic Acid + Propionic Acid + Solvent (Amyl Alcohol, Cyclohexyl Acetate, or Toluene) Systems |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.44507e+01 |
| Coeff. B | -3.61094e+03 |
| Coeff. C | -7.90080e+01 |
| Temperature range (K), min. | 333.96 |
| Temperature range (K), max. | 474.11 |

# Sources

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| **(Liquid + liquid) equilibria of (water + butyric acid + cyclohexyl acetate) ternary systems:** | https://www.doi.org/10.1016/j.jct.2004.09.002 |
| **Phase equilibria for ternary liquid systems of (water + levulinic acid + cyclic solvent) at T = 298.2 K:** | https://www.doi.org/10.1016/j.jct.2005.01.014 |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Thermodynamic modeling:** | |
| **Liquid-liquid equilibria study of the (water + phosphoric acid + hexyl or cyclohexyl acetate) systems at T = (298.15, 308.15, and 318.15) K:** | https://www.doi.org/10.1016/j.jct.2016.03.025 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Measurement and thermodynamic modelling:** | |
| **Quaternary Liquid-Liquid Equilibrium of Water + Acetic Acid + Propionic Acid + Solvent (Amyl Alcohol, Cyclohexyl Acetate, or Toluene) Systems:** | https://www.doi.org/10.1021/je049848j |
| **Solubility of fragrance raw materials in water: Experimental study, Correlations, and Mod. UNIFAC (Do) Predictions:** | https://www.doi.org/10.1016/j.jct.2010.07.013 |
| **Combustion, Solubility, and Sublimation Energetics and Enthalpies of Vaporization of Cyclohexyl Esters:** | https://www.doi.org/10.1021/je025634v |
| **Phase equilibria of water + 1-propanol + solvent (n-amyl acetate, cyclohexanol, and cyclohexyl acetate) at T = 298.2 K:** | https://www.doi.org/10.1016/j.fluid.2007.01.021 |
| **Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material):** | https://www.doi.org/10.1016/j.tca.2009.02.013 |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Phase Equilibria for the Ternary Liquid Systems of (Water + Tetrahydrofurfuryl Alcohol + Cyclic Solvent) at 298.2 K:** | https://www.doi.org/10.1021/je049605r |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C622457&Units=SI |

# Legend

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|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rfi:** | Refractive Index |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |

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|---|---|
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |