

Acetic acid, cyclohexyl ester

Other names:	Acetoxy cyclohexane 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	1024.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1043.00		NIST Webbook

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rinpol	1043.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	999.00		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	309.24	J/mol×K	584.06	Joback Method
cpg	323.01	J/mol×K	619.32	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	348.27	J/mol×K	689.84	Joback Method
cpg	336.02	J/mol×K	654.58	Joback Method

dvisc	0.0011600	Paxs	330.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)
dvisc	0.0013600	Paxs	320.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)
dvisc	0.0016100	Paxs	310.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)
dvisc	0.0019500	Paxs	300.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)
dvisc	0.0010100	Paxs	340.00	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	1.44250	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
rfi	1.44100	293.20	Phase Equilibria for the Ternary Liquid Systems of (Water + Tetrahydrofurfuryl Alcohol + Cyclic Solvent) at 298.2 K

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

Phase equilibria of water + 1-propanol + solvent (n-amyl acetate, cyclohexane, and cyclohexyl acetate) at T = 298.2 K: Joback Method:	https://www.doi.org/10.1016/j.fluid.2007.01.021
Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C622457&Units=SI
Quaternary Liquid-Liquid Equilibrium of Water + Acetic Acid + Propionic Acid + Solvent (Aromatic, polar, nonpolar, dependent on the density and viscosity of binary mixtures of the water + phosphoric acid + hexyl or cyclohexyl acetate) at T = Pressure and End of process (T = Pressure and End of process): Measurement and thermodynamic prediction:	https://en.wikipedia.org/wiki/Joback_method
Phase Equilibria for the Ternary Liquid Systems of (Water + Tetrahydrofurfuryl Alcohol + Cyclic Solvent) at 298.2 K + butyric acid + cyclohexyl acetate) Aqueous Solubility Prediction Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
McGowan Method:	https://www.doi.org/10.1021/je049848j
Solubility of fragrance raw materials in water: Experimental study, Phase equilibria of ternary (Dio) systems of (water + levulinic acid + cyclic solvent) at T = 298.2 K: Thermodynamic modeling:	https://www.doi.org/10.1016/j.tca.2009.02.013
https://www.doi.org/10.1016/j.jct.2016.03.025	https://www.doi.org/10.1016/j.jct.2016.03.025
https://www.doi.org/10.1021/je025634v	https://www.doi.org/10.1021/je025634v
https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure-prediction	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure-prediction
https://www.doi.org/10.1021/je049605r	https://www.doi.org/10.1021/je049605r
https://www.doi.org/10.1016/j.jct.2004.09.002	https://www.doi.org/10.1016/j.jct.2004.09.002
http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
http://link.springer.com/article/10.1007/BF02311772	http://link.springer.com/article/10.1007/BF02311772
https://www.doi.org/10.1016/j.jct.2010.07.013	https://www.doi.org/10.1016/j.jct.2010.07.013
https://www.doi.org/10.1016/j.jct.2005.01.014	https://www.doi.org/10.1016/j.jct.2005.01.014

Legend

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
rinp0l:	Non-polar retention indices
rip0l:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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