2-CYCLOHEXYLETHYL ACETATE

Other names:	Acetic acid, cyclohexylethyl ester
	Cyclohexane ethyl acetate
	Cyclohexylethyl acetate
	Ethylcyclohexyl acetate
	Hexahydrophenyl ethyl acetate
Inchi:	InChI=1S/C10H18O2/c1-9(11)12-8-7-10-5-3-2-4-6-10/h10H,2-8H2,1H3
InchiKey:	NOTFZGFABLVTIG-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CC(=O)OCCC1CCCCC1
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
af	0.4485		Cheméo Relay (1.0)
gf	-176.15	kJ/mol	Joback Method
hf	-531.09	kJ/mol	Cheméo Relay (1.0)
hfus	16.28	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Cheméo Relay (1.0)
ie	9.46	eV	Cheméo Relay (1.0)
log10ws	-2.99		Cheméo Relay (1.0)
logp	2.520		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1233.00		NIST Webbook
rinpol	1233.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1591.00		NIST Webbook
tb	501.41	K	Cheméo Relay (1.0)
tc	702.21	K	Cheméo Relay (1.0)
tf	237.34	K	Cheméo Relay (1.0)
vc	0.524	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.31	J/mol×K	524.04	Joback Method
cpg	373.16	J/mol×K	558.27	Joback Method
cpg	390.11	J/mol×K	592.49	Joback Method
cpg	406.18	J/mol×K	626.72	Joback Method
cpg	421.39	J/mol×K	660.94	Joback Method
cpg	435.73	J/mol×K	695.17	Joback Method
cpg	449.24	J/mol×K	729.39	Joback Method
dvisc	0.0025400	Pa×s	300.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)
dvisc	0.0020700	Pa×s	310.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)
dvisc	0.0017200	Pa×s	320.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)
dvisc	0.0014600	Pa×s	330.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)
dvisc	0.0012600	Pa×s	340.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.70	K	2.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21722838&Units=SI
Cheméo Relay (1.0):	
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume