Cyclohexaneacetic acid

Other names: acetic acid, cyclohexyl-
cyclohexylacetic acid
cyclohexylethanoic acid
Inchi: InChI=1S/C8H14O2/c9-8(10)6-7-4-2-1-3-5-7/h7H,1-6H2,(H,9,10)
InchiKey: LJOODBDWMQKMFB-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: O=C(O)CC1CCCCC1
Mol. weight [g/mol]: 142.20
CAS: 5292-21-7

Physical Properties

Property code	Value	Unit	Source
gf	-224.81	kJ/mol	Joback Method
hf	-418.94	kJ/mol	Joback Method
hfus	14.00	kJ/mol	Joback Method
hvap	57.26	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	2.041		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	516.20	K	NIST Webbook
tb	518.20	K	NIST Webbook
tc	747.55	K	Joback Method
tf	300.00 ± 4.00	K	NIST Webbook
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.11	J/mol×K	747.55	Joback Method
cpg	356.93	J/mol×K	714.30	Joback Method
cpg	346.08	J/mol×K	681.05	Joback Method
cpg	334.54	J/mol×K	647.80	Joback Method
cpg	322.29	J/mol×K	614.54	Joback Method

cpg	309.31	J/mol×K	581.29	Joback Method
cpg	295.58	J/mol×K	548.04	Joback Method
dvisc	0.0181618	Pa×s	298.05	Joback Method
dvisc	0.0001455	Pa×s	548.04	Joback Method
dvisc	0.0002337	Pa×s	506.38	Joback Method
dvisc	0.0004084	Pa×s	464.71	Joback Method
dvisc	0.0007968	Pa×s	423.04	Joback Method
dvisc	0.0017992	Pa×s	381.38	Joback Method
dvisc	0.0049607	Pa×s	339.72	Joback Method
hfust	13.80	kJ/mol	302.60	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	1.70	NIST Webbook

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5292217&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume