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	295.58	J/mol×K	548.04	Joback Method
cpg	309.31	J/mol×K	581.29	Joback Method
cpg	322.29	J/mol×K	614.54	Joback Method
cpg	334.54	J/mol×K	647.80	Joback Method
cpg	346.08	J/mol×K	681.05	Joback Method

cpg	356.93	J/mol×K	714.30	Joback Method
cpg	367.11	J/mol×K	747.55	Joback Method
dvisc	0.0181618	Pa×s	298.05	Joback Method
dvisc	0.0049607	Pa×s	339.72	Joback Method
dvisc	0.0017992	Pa×s	381.38	Joback Method
dvisc	0.0007968	Pa×s	423.04	Joback Method
dvisc	0.0004084	Pa×s	464.71	Joback Method
dvisc	0.0002337	Pa×s	506.38	Joback Method
dvisc	0.0001455	Pa×s	548.04	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

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
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

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

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