CYCLOHEXANEPROPIONIC ACID

Other names:	Cyclohexanepropionic acid
	3-Cyclohexanepropionic acid
	3-Cyclohexylpropanoic acid
	3-Cyclohexylpropionic acid
	«beta»-Cyclohexylpropionic acid
	Cyclohexylpropionic acid
Inchi:	InChI=1S/C9H16O2/c10-9(11)7-6-8-4-2-1-3-5-8/h8H,1-7H2,(H,10,11)
InchiKey:	HJZLEGIHUQOJBA-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	O=C(O)CCC1CCCCC1
Mol. weight [g/mol]:	156.23

Physical Properties

Property code	Value	Unit	Source
af	0.6635		Cheméo Relay (1.0)
gf	-216.39	kJ/mol	Joback Method
hf	-546.89	kJ/mol	Cheméo Relay (1.0)
hfus	16.59	kJ/mol	Joback Method
hvap	82.05	kJ/mol	Cheméo Relay (1.0)
ie	9.80	eV	Cheméo Relay (1.0)
log10ws	-2.19		Cheméo Relay (1.0)
logp	2.432		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
tb	549.70	K	NIST Webbook
tc	748.60	K	Cheméo Relay (1.0)
tf	312.50	K	Cheméo Relay (1.0)
vc	0.454	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.92	J/mol×K	570.92	Joback Method
cpg	357.38	J/mol×K	603.71	Joback Method

cpg	371.05	J/mol×K	636.51	Joback Method
cpg	383.96	J/mol×K	669.30	Joback Method
cpg	396.12	J/mol×K	702.10	Joback Method
cpg	407.56	J/mol×K	734.89	Joback Method
cpg	418.31	J/mol×K	767.69	Joback Method
dvisc	0.0150786	Pa×s	309.32	Joback Method
dvisc	0.0041209	Pa×s	352.92	Joback Method
dvisc	0.0014980	Pa×s	396.52	Joback Method
dvisc	0.0006654	Pa×s	440.12	Joback Method
dvisc	0.0003422	Pa×s	483.72	Joback Method
dvisc	0.0001964	Pa×s	527.32	Joback Method
dvisc	0.0001227	Pa×s	570.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C701973&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume