

Cyclohexanecarboxylic acid, 2-hydroxy-, methyl ester

Other names:	methyl 2-hydroxycyclohexanecarboxylate
Inchi:	InChI=1S/C8H14O3/c1-11-8(10)6-4-2-3-5-7(6)9/h6-7,9H,2-5H2,1H3
InchiKey:	IAJQZEQYGUQTQS-UHFFFAOYSA-N
Formula:	C8H14O3
SMILES:	COC(=O)C1CCCCC1O
Mol. weight [g/mol]:	158.19
CAS:	2236-11-5

Physical Properties

Property code	Value	Unit	Source
gf	-337.52	kJ/mol	Joback Method
hf	-571.50	kJ/mol	Joback Method
hfus	16.26	kJ/mol	Joback Method
hvap	59.36	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.710		Crippen Method
mcvol	126.030	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
tb	565.79	K	Joback Method
tc	763.42	K	Joback Method
tf	316.04	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.94	J/mol×K	565.79	Joback Method
cpg	335.79	J/mol×K	598.73	Joback Method
cpg	348.96	J/mol×K	631.67	Joback Method
cpg	361.43	J/mol×K	664.60	Joback Method
cpg	373.23	J/mol×K	697.54	Joback Method
cpg	384.34	J/mol×K	730.48	Joback Method
cpg	394.77	J/mol×K	763.42	Joback Method
dvisc	0.0085780	Pa×s	316.04	Joback Method

dvisc	0.0028126	Pa×s	357.67	Joback Method
dvisc	0.0011636	Pa×s	399.29	Joback Method
dvisc	0.0005687	Pa×s	440.91	Joback Method
dvisc	0.0003145	Pa×s	482.54	Joback Method
dvisc	0.0001910	Pa×s	524.16	Joback Method
dvisc	0.0001249	Pa×s	565.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2236115&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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