2-Hydroxy-cyclohexanecarboxylic acid ethyl ester, cis

Inchi: InChI=1S/C9H16O3/c1-2-12-9(11)7-5-3-4-6-8(7)10/h7-8,10H,2-6H2,1H3/t7-,8+/m1/s1
InchiKey: WOGRTPJVNNCUKN-SFYZADRCSA-N
Formula: C9H16O3
SMILES: CCOC(=O)C1CCCCC1O
Mol. weight [g/mol]: 172.22

Physical Properties

Property code	Value	Unit	Source
gf	-329.10	kJ/mol	Joback Method
hf	-592.14	kJ/mol	Joback Method
hfus	18.85	kJ/mol	Joback Method
hvap	61.58	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.101		Crippen Method
mcvol	140.120	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1189.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1263.00		NIST Webbook
tb	588.67	K	Joback Method
tc	783.67	K	Joback Method
tf	327.31	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.23	J/mol×K	588.67	Joback Method
cpg	435.77	J/mol×K	751.17	Joback Method
cpg	424.12	J/mol×K	718.67	Joback Method
cpg	411.74	J/mol×K	686.17	Joback Method
cpg	398.64	J/mol×K	653.67	Joback Method
cpg	384.80	J/mol×K	621.17	Joback Method
cpg	446.71	J/mol×K	783.67	Joback Method

dvisc	0.0001062	Pa×s	588.67	Joback Method
dvisc	0.0001623	Pa×s	545.11	Joback Method
dvisc	0.0002668	Pa×s	501.55	Joback Method
dvisc	0.0004824	Pa×s	457.99	Joback Method
dvisc	0.0009877	Pa×s	414.43	Joback Method
dvisc	0.0023928	Pa×s	370.87	Joback Method
dvisc	0.0073369	Pa×s	327.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136680&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume