

2-Hydroxy-cyclopentanecarboxylic acid ethyl ester, cis

Inchi:	InChI=1S/C8H14O3/c1-2-11-8(10)6-4-3-5-7(6)9/h6-7,9H,2-5H2,1H3/t6-,7+/m0/s1
InchiKey:	IIFIGGNBUOZGAB-NKWVEPMBSA-N
Formula:	C8H14O3
SMILES:	CCOC(=O)C1CCCC1O
Mol. weight [g/mol]:	158.19

Physical Properties

Property code	Value	Unit	Source
gf	-325.42	kJ/mol	Joback Method
hf	-565.34	kJ/mol	Joback Method
hfus	18.36	kJ/mol	Joback Method
hvap	59.19	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.710		Crippen Method
mcvol	126.030	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	1162.00		NIST Webbook
rinpol	1098.00		NIST Webbook
tb	561.52	K	Joback Method
tc	752.76	K	Joback Method
tf	319.56	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.27	J/molxK	561.52	Joback Method
cpg	334.32	J/molxK	593.39	Joback Method
cpg	346.74	J/molxK	625.27	Joback Method
cpg	358.54	J/molxK	657.14	Joback Method
cpg	369.73	J/molxK	689.02	Joback Method
cpg	380.30	J/molxK	720.89	Joback Method
cpg	390.28	J/molxK	752.76	Joback Method
dvisc	0.0072063	Paxs	319.56	Joback Method

dvisc	0.0026857	Paxs	359.89	Joback Method
dvisc	0.0012212	Paxs	400.21	Joback Method
dvisc	0.0006415	Paxs	440.54	Joback Method
dvisc	0.0003754	Paxs	480.87	Joback Method
dvisc	0.0002387	Paxs	521.19	Joback Method
dvisc	0.0001619	Paxs	561.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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

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