

2-Hydroxy-cyclopentanecarboxylic acid ethyl ester, trans

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-BQBZGAKWSA-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	1106.00		NIST Webbook
rinpol	1180.00		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	380.30	J/molxK	720.89	Joback Method
cpg	369.73	J/molxK	689.02	Joback Method
cpg	358.54	J/molxK	657.14	Joback Method
cpg	346.74	J/molxK	625.27	Joback Method
cpg	334.32	J/molxK	593.39	Joback Method
cpg	390.28	J/molxK	752.76	Joback Method
dvisc	0.0001619	Paxs	561.52	Joback Method

dvisc	0.0002387	Paxs	521.19	Joback Method
dvisc	0.0003754	Paxs	480.87	Joback Method
dvisc	0.0006415	Paxs	440.54	Joback Method
dvisc	0.0012212	Paxs	400.21	Joback Method
dvisc	0.0026857	Paxs	359.89	Joback Method
dvisc	0.0072063	Paxs	319.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136739&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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