Propanoic acid, 2-amino-3-hydroxy, propyl ester

Inchi: InChI=1S/C6H13NO3/c1-2-3-10-6(9)5(7)4-8/h5,8H,2-4,7H2,1H3
InchiKey: VZNRCOQNPQNNKI-UHFFFAOYSA-N
Formula: C6H13NO3
SMILES: CCCOC(=O)C(N)CO
Mol. weight [g/mol]: 147.17

Physical Properties

Property code	Value	Unit	Source
gf	-307.09	kJ/mol	Joback Method
hf	-535.69	kJ/mol	Joback Method
hfus	19.85	kJ/mol	Joback Method
hvap	65.04	kJ/mol	Joback Method
log10ws	-6.09e-03		Crippen Method
logp	-0.741		Crippen Method
mcvol	118.690	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
rinpol	1195.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1200.00		NIST Webbook
tb	577.24	K	Joback Method
tc	761.34	K	Joback Method
tf	358.62	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.68	J/mol×K	577.24	Joback Method
cpg	307.06	J/mol×K	607.92	Joback Method
cpg	316.03	J/mol×K	638.61	Joback Method
cpg	324.59	J/mol×K	669.29	Joback Method
cpg	332.74	J/mol×K	699.97	Joback Method

cpg	340.49	J/mol×K	730.65	Joback Method
cpg	347.83	J/mol×K	761.34	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R535903&Units=SI

Legend

cpg:	Ideal gas heat capacity
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