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

Inchi: InChI=1S/C7H15NO3/c1-3-4-11-7(10)6(8)5(2)9/h5-6,9H,3-4,8H2,1-2H3
InchiKey: RELVKKXAEWOJGJ-UHFFFAOYSA-N
Formula: C7H15NO3
SMILES: CCCOC(=O)C(N)C(C)O
Mol. weight [g/mol]: 161.20

Physical Properties

Property code	Value	Unit	Source
gf	-301.11	kJ/mol	Joback Method
hf	-561.61	kJ/mol	Joback Method
hfus	18.91	kJ/mol	Joback Method
hvap	66.88	kJ/mol	Joback Method
log10ws	-0.54		Crippen Method
logp	-0.352		Crippen Method
mcvol	132.780	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	1165.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1180.00		NIST Webbook
tb	599.68	K	Joback Method
tc	785.25	K	Joback Method
tf	354.89	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.26	J/mol×K	599.68	Joback Method
cpg	354.74	J/mol×K	630.61	Joback Method
cpg	364.73	J/mol×K	661.54	Joback Method
cpg	374.25	J/mol×K	692.47	Joback Method
cpg	383.28	J/mol×K	723.40	Joback Method

cpg	391.85	J/mol×K	754.33	Joback Method
cpg	399.94	J/mol×K	785.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R535829&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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