dl-Threonine, methyl ester

Other names: Butanoic acid, 2-amino-3-hydroxy, methyl ester
Inchi: InChI=1S/C5H11NO3/c1-3(7)4(6)5(8)9-2/h3-4,7H,6H2,1-2H3
InchiKey: TVHCXXXXQNWQLP-UHFFFAOYSA-N
Formula: C5H11NO3
SMILES: COC(=O)C(N)C(C)O
Mol. weight [g/mol]: 133.15

Physical Properties

Property code	Value	Unit	Source
gf	-317.95	kJ/mol	Joback Method
hf	-520.33	kJ/mol	Joback Method
hfus	13.73	kJ/mol	Joback Method
hvap	62.42	kJ/mol	Joback Method
log10ws	0.30		Crippen Method
logp	-1.132		Crippen Method
mcvol	104.600	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
rinpol	1043.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1043.00		NIST Webbook
tb	553.92	K	Joback Method
tc	743.70	K	Joback Method
tf	332.35	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.76	J/mol×K	553.92	Joback Method
cpg	262.39	J/mol×K	585.55	Joback Method
cpg	270.65	J/mol×K	617.18	Joback Method
cpg	278.52	J/mol×K	648.81	Joback Method
cpg	286.01	J/mol×K	680.44	Joback Method

cpg	293.12	J/mol×K	712.07	Joback Method
cpg	299.86	J/mol×K	743.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U130332&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