l-Methionine, N-pivaloyl-, methyl ester

Inchi: InChI=1S/C11H21NO3S/c1-11(2,3)10(14)12-8(6-7-16-5)9(13)15-4/h8H,6-7H2,1-5H3,(H,1
InchiKey: UKXONFCTNLUFPB-UHFFFAOYSA-N
Formula: C11H21NO3S
SMILES: COC(=O)C(CCSC)NC(=O)C(C)(C)C
Mol. weight [g/mol]: 247.35

Physical Properties

Property code	Value	Unit	Source
gf	-198.19	kJ/mol	Joback Method
hf	-546.44	kJ/mol	Joback Method
hfus	26.92	kJ/mol	Joback Method
hvap	67.55	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.443		Crippen Method
mcvol	201.190	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
tb	696.52	K	Joback Method
tc	904.85	K	Joback Method
tf	410.30	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.22	J/mol×K	696.52	Joback Method
cpg	566.68	J/mol×K	731.24	Joback Method
cpg	580.20	J/mol×K	765.96	Joback Method
cpg	592.80	J/mol×K	800.69	Joback Method
cpg	604.53	J/mol×K	835.41	Joback Method
cpg	615.39	J/mol×K	870.13	Joback Method
cpg	625.43	J/mol×K	904.85	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=U299747&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