l-Methionine, N-capryloyl-, methyl ester

Inchi: InChI=1S/C14H27NO3S/c1-4-5-6-7-8-9-13(16)15-12(10-11-19-3)14(17)18-2/h12H,4-11H
InchiKey: DHRWESWFXFVTLO-UHFFFAOYSA-N
Formula: C14H27NO3S
SMILES: CCCCCCCC(=O)NC(CCSC)C(=O)OC
Mol. weight [g/mol]: 289.43

Physical Properties

Property code	Value	Unit	Source
gf	-175.77	kJ/mol	Joback Method
hf	-599.61	kJ/mol	Joback Method
hfus	42.11	kJ/mol	Joback Method
hvap	75.53	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	2.758		Crippen Method
mcvol	243.460	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	2106.00		NIST Webbook
rinpol	2106.00		NIST Webbook
tb	768.39	K	Joback Method
tc	963.32	K	Joback Method
tf	441.69	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.80	J/mol×K	768.39	Joback Method
cpg	729.01	J/mol×K	800.88	Joback Method
cpg	743.27	J/mol×K	833.37	Joback Method
cpg	756.60	J/mol×K	865.85	Joback Method
cpg	769.03	J/mol×K	898.34	Joback Method
cpg	780.55	J/mol×K	930.83	Joback Method
cpg	791.19	J/mol×K	963.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299727&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

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