l-Methionine, N-caproyl-, methyl ester

Inchi: InChI=1S/C12H23NO3S/c1-4-5-6-7-11(14)13-10(8-9-17-3)12(15)16-2/h10H,4-9H2,1-3H3
InchiKey: FFRRQECVACLCBP-UHFFFAOYSA-N
Formula: C12H23NO3S
SMILES: CCCCCC(=O)NC(CCSC)C(=O)OC
Mol. weight [g/mol]: 261.38

Physical Properties

Property code	Value	Unit	Source
gf	-192.61	kJ/mol	Joback Method
hf	-558.33	kJ/mol	Joback Method
hfus	36.93	kJ/mol	Joback Method
hvap	71.07	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	1.978		Crippen Method
mcvol	215.280	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1902.00		NIST Webbook
tb	722.63	K	Joback Method
tc	919.66	K	Joback Method
tf	419.15	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.12	J/mol×K	722.63	Joback Method
cpg	617.61	J/mol×K	755.47	Joback Method
cpg	631.23	J/mol×K	788.31	Joback Method
cpg	644.00	J/mol×K	821.14	Joback Method
cpg	655.92	J/mol×K	853.98	Joback Method
cpg	667.02	J/mol×K	886.82	Joback Method
cpg	677.28	J/mol×K	919.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299736&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