l-Methionine, N-(3-cyclopentylpropionyl)-, methyl ester

Inchi: InChI=1S/C14H25NO3S/c1-18-14(17)12(9-10-19-2)15-13(16)8-7-11-5-3-4-6-11/h11-12H

InchiKey: ACKLGNFAPITYLJ-UHFFFAOYSA-N

Formula: C14H25NO3S

SMILES: COC(=O)C(CCSC)NC(=O)CCC1CCCC1

Mol. weight [g/mol]: 287.42

Physical Properties

Property code	Value	Unit	Source
gf	-139.22	kJ/mol	Joback Method
hf	-539.13	kJ/mol	Joback Method
hfus	36.04	kJ/mol	Joback Method
hvap	75.78	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.368		Crippen Method
mcvol	232.600	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2182.00		NIST Webbook
rinpol	2182.00		NIST Webbook
tb	783.67	K	Joback Method
tc	997.21	K	Joback Method
tf	452.59	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.55	J/mol×K	783.67	Joback Method
cpg	720.80	J/mol×K	819.26	Joback Method
cpg	735.85	J/mol×K	854.85	Joback Method
cpg	749.73	J/mol×K	890.44	Joback Method
cpg	762.48	J/mol×K	926.03	Joback Method
cpg	774.12	J/mol×K	961.62	Joback Method
cpg	784.67	J/mol×K	997.21	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=U299655&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