Sarcosine, N-valeryl-, hexyl ester

Inchi: InChI=1S/C14H27NO3/c1-4-6-8-9-11-18-14(17)12-15(3)13(16)10-7-5-2/h4-12H2,1-3H3
InchiKey: PMUACKSSIGXLNX-UHFFFAOYSA-N
Formula: C14H27NO3
SMILES: CCCCCCOC(=O)CN(C)C(=O)CCCC
Mol. weight [g/mol]: 257.37

Physical Properties

Property code	Value	Unit	Source
gf	-185.06	kJ/mol	Joback Method
hf	-622.14	kJ/mol	Joback Method
hfus	39.42	kJ/mol	Joback Method
hvap	64.70	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.758		Crippen Method
mcvol	227.110	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	1913.00		NIST Webbook
tb	662.32	K	Joback Method
tc	837.24	K	Joback Method
tf	402.10	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.14	J/mol×K	662.32	Joback Method
cpg	649.26	J/mol×K	691.47	Joback Method
cpg	664.62	J/mol×K	720.63	Joback Method
cpg	679.22	J/mol×K	749.78	Joback Method
cpg	693.08	J/mol×K	778.93	Joback Method
cpg	706.23	J/mol×K	808.08	Joback Method
cpg	718.68	J/mol×K	837.24	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=U321564&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