Sarcosine, N-valeryl-, isohexyl ester

Inchi: InChI=1S/C14H27NO3/c1-5-6-9-13(16)15(4)11-14(17)18-10-7-8-12(2)3/h12H,5-11H2,1-4
InchiKey: FLTRRMZRPBGRHB-UHFFFAOYSA-N
Formula: C14H27NO3
SMILES: CCCCC(=O)N(C)CC(=O)OCCCC(C)C
Mol. weight [g/mol]: 257.37

Physical Properties

Property code	Value	Unit	Source
gf	-187.50	kJ/mol	Joback Method
hf	-627.42	kJ/mol	Joback Method
hfus	35.90	kJ/mol	Joback Method
hvap	64.31	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.614		Crippen Method
mcvol	227.110	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	661.88	K	Joback Method
tc	839.22	K	Joback Method
tf	387.10	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.58	J/mol×K	661.88	Joback Method
cpg	649.96	J/mol×K	691.44	Joback Method
cpg	665.54	J/mol×K	720.99	Joback Method
cpg	680.34	J/mol×K	750.55	Joback Method
cpg	694.38	J/mol×K	780.11	Joback Method
cpg	707.67	J/mol×K	809.66	Joback Method
cpg	720.24	J/mol×K	839.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321563&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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