Sarcosylsarcosine, N-isobutoxycarbonyl-, propyl ester

Inchi: InChI=1S/C14H26N2O5/c1-6-7-20-13(18)9-15(4)12(17)8-16(5)14(19)21-10-11(2)3/h11H
InchiKey: ZJEQLWFJQXQOOA-UHFFFAOYSA-N
Formula: C14H26N2O5
SMILES: CCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCC(C)C
Mol. weight [g/mol]: 302.37

Physical Properties

Property code	Value	Unit	Source
gf	-310.64	kJ/mol	Joback Method
hf	-804.69	kJ/mol	Joback Method
hfus	41.71	kJ/mol	Joback Method
hvap	75.51	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	1.122		Crippen Method
mcvol	244.530	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	2099.00		NIST Webbook
tb	750.61	K	Joback Method
tc	935.37	K	Joback Method
tf	491.73	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.55	J/mol×K	750.61	Joback Method
cpg	740.54	J/mol×K	781.40	Joback Method
cpg	754.63	J/mol×K	812.20	Joback Method
cpg	767.85	J/mol×K	842.99	Joback Method
cpg	780.22	J/mol×K	873.78	Joback Method
cpg	791.73	J/mol×K	904.57	Joback Method
cpg	802.43	J/mol×K	935.37	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=U320578&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