Sarcosylsarcosine, N-isobutoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C18H34N2O5/c1-6-7-8-9-10-11-24-17(22)13-19(4)16(21)12-20(5)18(23)25-14-

InchiKey: NABAISOCMVPTDI-UHFFFAOYSA-N

Formula: C18H34N2O5

SMILES: CCCCCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCC(C)C

Mol. weight [g/mol]: 358.47

Physical Properties

Property code	Value	Unit	Source
gf	-276.96	kJ/mol	Joback Method
hf	-887.25	kJ/mol	Joback Method
hfus	52.07	kJ/mol	Joback Method
hvap	84.42	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.683		Crippen Method
mcvol	300.890	ml/mol	McGowan Method
pc	1287.44	kPa	Joback Method
rinpol	2423.00		NIST Webbook
tb	842.13	K	Joback Method
tc	1033.46	K	Joback Method
tf	536.81	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.98	J/mol×K	842.13	Joback Method
cpg	974.35	J/mol×K	874.02	Joback Method
cpg	989.63	J/mol×K	905.91	Joback Method
cpg	1003.85	J/mol×K	937.80	Joback Method
cpg	1017.03	J/mol×K	969.69	Joback Method
cpg	1029.20	J/mol×K	1001.58	Joback Method
cpg	1040.38	J/mol×K	1033.46	Joback Method

Sources

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=U320582&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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