Sarcosylsarcosine, n-butoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C17H32N2O5/c1-6-7-10-24-17(22)19(5)12-15(20)18(4)13-16(21)23-11-8-9-14(

InchiKey: DFNNQGRUJRJXNM-UHFFFAOYSA-N

Formula: C17H32N2O5

SMILES: CCCCOC(=O)N(C)CC(=O)N(C)CC(=O)OCCCC(C)C

Mol. weight [g/mol]: 344.45

Physical Properties

Property code	Value	Unit	Source
gf	-285.38	kJ/mol	Joback Method
hf	-866.61	kJ/mol	Joback Method
hfus	49.48	kJ/mol	Joback Method
hvap	82.19	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.293		Crippen Method
mcvol	286.800	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	2350.00		NIST Webbook
tb	819.25	K	Joback Method
tc	1007.89	K	Joback Method
tf	525.54	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.59	J/mol×K	819.25	Joback Method
cpg	914.62	J/mol×K	850.69	Joback Method
cpg	929.61	J/mol×K	882.13	Joback Method
cpg	943.60	J/mol×K	913.57	Joback Method
cpg	956.59	J/mol×K	945.01	Joback Method
cpg	968.63	J/mol×K	976.45	Joback Method
cpg	979.73	J/mol×K	1007.89	Joback Method

Sources

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=U320665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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