Sarcosylsarcosine, n-butoxycarbonyl-, hexyl ester

Inchi: InChI=1S/C17H32N2O5/c1-5-7-9-10-12-23-16(21)14-18(3)15(20)13-19(4)17(22)24-11-8-

InchiKey: WMGCLQYMQNSQOF-UHFFFAOYSA-N

Formula: C17H32N2O5

SMILES: CCCCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCCCC

Mol. weight [g/mol]: 344.45

Physical Properties

Property code	Value	Unit	Source
gf	-282.94	kJ/mol	Joback Method
hf	-861.33	kJ/mol	Joback Method
hfus	53.00	kJ/mol	Joback Method
hvap	82.58	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.437		Crippen Method
mcvol	286.800	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2393.00		NIST Webbook
rinpol	2393.00		NIST Webbook
tb	819.69	K	Joback Method
tc	1007.36	K	Joback Method
tf	540.54	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.08	J/mol×K	819.69	Joback Method
cpg	914.03	J/mol×K	850.97	Joback Method
cpg	928.96	J/mol×K	882.25	Joback Method
cpg	942.90	J/mol×K	913.52	Joback Method
cpg	955.88	J/mol×K	944.80	Joback Method
cpg	967.91	J/mol×K	976.08	Joback Method
cpg	979.02	J/mol×K	1007.36	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=U320666&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