Sarcosylsarcosine, N-ethoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C15H28N2O5/c1-6-21-15(20)17(5)10-13(18)16(4)11-14(19)22-9-7-8-12(2)3/h1

InchiKey: LKGMQIGSVUYJAL-UHFFFAOYSA-N

Formula: C15H28N2O5

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

Mol. weight [g/mol]: 316.39

Physical Properties

Property code	Value	Unit	Source
gf	-302.22	kJ/mol	Joback Method
hf	-825.33	kJ/mol	Joback Method
hfus	44.30	kJ/mol	Joback Method
hvap	77.74	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.512		Crippen Method
mcvol	258.620	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	2186.00		NIST Webbook
tb	773.49	K	Joback Method
tc	958.90	K	Joback Method
tf	503.00	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.31	J/mol×K	773.49	Joback Method
cpg	797.65	J/mol×K	804.39	Joback Method
cpg	812.05	J/mol×K	835.29	Joback Method
cpg	825.55	J/mol×K	866.19	Joback Method
cpg	838.14	J/mol×K	897.09	Joback Method
cpg	849.85	J/mol×K	928.00	Joback Method
cpg	860.71	J/mol×K	958.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320691&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

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