

Sarcosylsarcosine, N-ethoxycarbonyl-, pentyl ester

Inchi:	InChI=1S/C14H26N2O5/c1-5-7-8-9-21-13(18)11-15(3)12(17)10-16(4)14(19)20-6-2/h5-11
InchiKey:	IZMYPFYCSLGMLP-UHFFFAOYSA-N
Formula:	C14H26N2O5
SMILES:	CCCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCC
Mol. weight [g/mol]:	302.37

Physical Properties

Property code	Value	Unit	Source
gf	-308.20	kJ/mol	Joback Method
hf	-799.41	kJ/mol	Joback Method
hfus	45.23	kJ/mol	Joback Method
hvap	75.90	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	1.266		Crippen Method
mcvol	244.530	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
tb	751.05	K	Joback Method
tc	933.94	K	Joback Method
tf	506.73	K	Joback Method
vc	0.909	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.02	J/mol×K	751.05	Joback Method
cpg	739.85	J/mol×K	781.53	Joback Method
cpg	753.81	J/mol×K	812.01	Joback Method
cpg	766.91	J/mol×K	842.50	Joback Method
cpg	779.19	J/mol×K	872.98	Joback Method
cpg	790.65	J/mol×K	903.46	Joback Method
cpg	801.30	J/mol×K	933.94	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=U320690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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