Sarcosylsarcosine, n-propoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C16H30N2O5/c1-6-9-23-16(21)18(5)11-14(19)17(4)12-15(20)22-10-7-8-13(2)3

InchiKey: YQVFRHSPXXMXGK-UHFFFAOYSA-N

Formula: C16H30N2O5

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

Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
gf	-293.80	kJ/mol	Joback Method
hf	-845.97	kJ/mol	Joback Method
hfus	46.89	kJ/mol	Joback Method
hvap	79.97	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.903		Crippen Method
mcvol	272.710	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	2266.00		NIST Webbook
tb	796.37	K	Joback Method
tc	983.05	K	Joback Method
tf	514.27	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.01	J/mol×K	796.37	Joback Method
cpg	855.70	J/mol×K	827.48	Joback Method
cpg	870.40	J/mol×K	858.60	Joback Method
cpg	884.14	J/mol×K	889.71	Joback Method
cpg	896.95	J/mol×K	920.83	Joback Method
cpg	908.83	J/mol×K	951.94	Joback Method
cpg	919.82	J/mol×K	983.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320638&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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