Sarcosylsarcosine, n-propoxycarbonyl-,dodecyl ester

Inchi: InChI=1S/C22H42N2O5/c1-5-7-8-9-10-11-12-13-14-15-17-28-21(26)19-23(3)20(25)18-24

InchiKey: JSUSYSZGLIWFNJ-UHFFFAOYSA-N

Formula: C22H42N2O5

SMILES: CCCCCCCCCCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCCC

Mol. weight [g/mol]: 414.58

Physical Properties

Property code	Value	Unit	Source
gf	-240.84	kJ/mol	Joback Method
hf	-964.53	kJ/mol	Joback Method
hfus	65.95	kJ/mol	Joback Method
hvap	93.71	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.387		Crippen Method
mcvol	357.250	ml/mol	McGowan Method
pc	989.51	kPa	Joback Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook
tb	934.09	K	Joback Method
tc	1145.70	K	Joback Method
tf	596.89	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1201.86	J/mol×K	934.09	Joback Method
cpg	1219.91	J/mol×K	969.36	Joback Method
cpg	1236.55	J/mol×K	1004.63	Joback Method
cpg	1251.81	J/mol×K	1039.89	Joback Method
cpg	1265.75	J/mol×K	1075.16	Joback Method
cpg	1278.42	J/mol×K	1110.43	Joback Method
cpg	1289.87	J/mol×K	1145.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320645&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