Sarcosine, n-hexanoyl-, dodecyl ester

Inchi: InChI=1S/C21H41NO3/c1-4-6-8-9-10-11-12-13-14-16-18-25-21(24)19-22(3)20(23)17-15-
InchiKey: OZGGKIZUGSDRKE-UHFFFAOYSA-N
Formula: C21H41NO3
SMILES: CCCCCCCCCCCCOC(=O)CN(C)C(=O)CCCCC
Mol. weight [g/mol]: 355.56

Physical Properties

Property code	Value	Unit	Source
gf	-126.12	kJ/mol	Joback Method
hf	-766.62	kJ/mol	Joback Method
hfus	57.55	kJ/mol	Joback Method
hvap	80.28	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.489		Crippen Method
mcvol	325.740	ml/mol	McGowan Method
pc	1022.69	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2608.00		NIST Webbook
tb	822.48	K	Joback Method
tc	1007.92	K	Joback Method
tf	480.99	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.80	J/mol×K	822.48	Joback Method
cpg	1060.87	J/mol×K	853.39	Joback Method
cpg	1078.86	J/mol×K	884.29	Joback Method
cpg	1095.82	J/mol×K	915.20	Joback Method
cpg	1111.78	J/mol×K	946.11	Joback Method
cpg	1126.76	J/mol×K	977.01	Joback Method
cpg	1140.82	J/mol×K	1007.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321128&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