Sarcosine, N-(cyclohexylcarbonyl)-, undecyl ester

Inchi: InChI=1S/C21H39NO3/c1-3-4-5-6-7-8-9-10-14-17-25-20(23)18-22(2)21(24)19-15-12-11-
InchiKey: ZXOBAQUKAIDUET-UHFFFAOYSA-N
Formula: C21H39NO3
SMILES: CCCCCCCCCCCOC(=O)CN(C)C(=O)C1CCCCC1
Mol. weight [g/mol]: 353.54

Physical Properties

Property code	Value	Unit	Source
gf	-101.67	kJ/mol	Joback Method
hf	-712.30	kJ/mol	Joback Method
hfus	49.39	kJ/mol	Joback Method
hvap	80.71	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	5.099		Crippen Method
mcvol	314.880	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	2668.00		NIST Webbook
rinpol	2668.00		NIST Webbook
tb	842.03	K	Joback Method
tc	1037.93	K	Joback Method
tf	488.37	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.48	J/mol×K	842.03	Joback Method
cpg	1059.01	J/mol×K	874.68	Joback Method
cpg	1077.25	J/mol×K	907.33	Joback Method
cpg	1094.24	J/mol×K	939.98	Joback Method
cpg	1110.04	J/mol×K	972.63	Joback Method
cpg	1124.67	J/mol×K	1005.28	Joback Method
cpg	1138.19	J/mol×K	1037.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321537&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