

Sarcosine, N-(cyclohexylcarbonyl)-, pentadecyl ester

Inchi:	InChI=1S/C25H47NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-18-21-29-24(27)22-26(2)25(28)
InchiKey:	KQEMPOFXGSHUBL-UHFFFAOYSA-N
Formula:	C25H47NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C1CCCCC1
Mol. weight [g/mol]:	409.65

Physical Properties

Property code	Value	Unit	Source
gf	-67.99	kJ/mol	Joback Method
hf	-794.86	kJ/mol	Joback Method
hfus	59.75	kJ/mol	Joback Method
hvap	89.62	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.659		Crippen Method
mcvol	371.240	ml/mol	McGowan Method
pc	914.94	kPa	Joback Method
tb	933.55	K	Joback Method
tc	1142.93	K	Joback Method
tf	533.45	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.19	J/molxK	933.55	Joback Method
cpg	1311.60	J/molxK	968.45	Joback Method
cpg	1330.49	J/molxK	1003.34	Joback Method
cpg	1347.92	J/molxK	1038.24	Joback Method
cpg	1363.97	J/molxK	1073.14	Joback Method
cpg	1378.69	J/molxK	1108.03	Joback Method
cpg	1392.15	J/molxK	1142.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321540&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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