

Sarcosine, N-(cyclohexylcarbonyl)-, hexadecyl ester

Inchi:	InChI=1S/C26H49NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-19-22-30-25(28)23-27(2)26(
InchiKey:	PJXRZCFOWNSHJJ-UHFFFAOYSA-N
Formula:	C26H49NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C1CCCCC1
Mol. weight [g/mol]:	423.67

Physical Properties

Property code	Value	Unit	Source
gf	-59.57	kJ/mol	Joback Method
hf	-815.50	kJ/mol	Joback Method
hfus	62.34	kJ/mol	Joback Method
hvap	91.84	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	7.050		Crippen Method
mvol	385.330	ml/mol	McGowan Method
pc	864.04	kPa	Joback Method
tb	956.43	K	Joback Method
tc	1171.51	K	Joback Method
tf	544.72	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1355.35	J/molxK	956.43	Joback Method
cpg	1376.08	J/molxK	992.28	Joback Method
cpg	1395.21	J/molxK	1028.12	Joback Method
cpg	1412.80	J/molxK	1063.97	Joback Method
cpg	1428.94	J/molxK	1099.82	Joback Method
cpg	1443.70	J/molxK	1135.67	Joback Method
cpg	1457.15	J/molxK	1171.51	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321541&Units=SI

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
mccvol:	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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