

Sarcosine, N-(3-cyclopentylpropionyl)-, pentadecyl ester

Inchi:	InChI=1S/C26H49NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-17-22-30-26(29)23-27(2)25(28)
InchiKey:	UKSCYKXLADVDCX-UHFFFAOYSA-N
Formula:	C26H49NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)CCC1CCCC1
Mol. weight [g/mol]:	423.67

Physical Properties

Property code	Value	Unit	Source
gf	-47.47	kJ/mol	Joback Method
hf	-809.34	kJ/mol	Joback Method
hfus	64.44	kJ/mol	Joback Method
hvap	91.67	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	7.050		Crippen Method
mcvol	385.330	ml/mol	McGowan Method
pc	851.47	kPa	Joback Method
tb	952.16	K	Joback Method
tc	1166.90	K	Joback Method
tf	548.24	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.78	J/molxK	952.16	Joback Method
cpg	1371.82	J/molxK	987.95	Joback Method
cpg	1391.35	J/molxK	1023.74	Joback Method
cpg	1409.47	J/molxK	1059.53	Joback Method
cpg	1426.25	J/molxK	1095.32	Joback Method
cpg	1441.78	J/molxK	1131.11	Joback Method
cpg	1456.14	J/molxK	1166.90	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=U321838&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
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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