

Sarcosine, N-(cyclopentylcarbonyl)-, hexadecyl ester

Inchi: InChI=1S/C25H47NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-29-24(27)22-26(2)25(28)23
InchiKey: DNAGEIMPLIQJPM-UHFFFAOYSA-N
Formula: C25H47NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C1CCCC1
Mol. weight [g/mol]: 409.65

Physical Properties

Property code	Value	Unit	Source
gf	-55.89	kJ/mol	Joback Method
hf	-788.70	kJ/mol	Joback Method
hfus	61.85	kJ/mol	Joback Method
hvap	89.45	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.659		Crippen Method
mcvol	371.240	ml/mol	McGowan Method
pc	901.26	kPa	Joback Method
tb	929.28	K	Joback Method
tc	1137.84	K	Joback Method
tf	536.97	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1286.55	J/mol×K	929.28	Joback Method
cpg	1307.15	J/mol×K	964.04	Joback Method
cpg	1326.33	J/mol×K	998.80	Joback Method
cpg	1344.16	J/mol×K	1033.56	Joback Method
cpg	1360.71	J/mol×K	1068.32	Joback Method
cpg	1376.06	J/mol×K	1103.08	Joback Method
cpg	1390.28	J/mol×K	1137.84	Joback Method

Sources

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=U321345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	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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