

Sarcosine, N-cyclopropylcarbonyl-, octadecyl ester

Inchi:	InChI=1S/C25H47NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-29-24(27)22-26
InchiKey:	PXNGDCKHOLPSCR-UHFFFAOYSA-N
Formula:	C25H47NO3
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C1CC1
Mol. weight [g/mol]:	409.65

Physical Properties

Property code	Value	Unit	Source
gf	-31.69	kJ/mol	Joback Method
hf	-776.38	kJ/mol	Joback Method
hfus	66.05	kJ/mol	Joback Method
hvap	89.10	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.659		Crippen Method
mcvol	371.240	ml/mol	McGowan Method
pc	874.80	kPa	Joback Method
tb	920.74	K	Joback Method
tc	1128.31	K	Joback Method
tf	544.01	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.19	J/molxK	920.74	Joback Method
cpg	1298.16	J/molxK	955.34	Joback Method
cpg	1317.89	J/molxK	989.93	Joback Method
cpg	1336.46	J/molxK	1024.53	Joback Method
cpg	1353.97	J/molxK	1059.12	Joback Method
cpg	1370.51	J/molxK	1093.72	Joback Method
cpg	1386.16	J/molxK	1128.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321201&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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