

Sarcosine, N-cyclopropylcarbonyl-, dodecyl ester

Inchi:	InChI=1S/C19H35NO3/c1-3-4-5-6-7-8-9-10-11-12-15-23-18(21)16-20(2)19(22)17-13-14-
InchiKey:	JCKNLUVDFCEYSX-UHFFFAOYSA-N
Formula:	C19H35NO3
SMILES:	CCCCCCCCCCCCOC(=O)CN(C)C(=O)C1CC1
Mol. weight [g/mol]:	325.49

Physical Properties

Property code	Value	Unit	Source
gf	-82.21	kJ/mol	Joback Method
hf	-652.54	kJ/mol	Joback Method
hfus	50.51	kJ/mol	Joback Method
hvap	75.75	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.319		Crippen Method
mcvol	286.700	ml/mol	McGowan Method
pc	1270.97	kPa	Joback Method
rinpol	2472.00		NIST Webbook
rinpol	2472.00		NIST Webbook
tb	783.46	K	Joback Method
tc	967.86	K	Joback Method
tf	476.39	K	Joback Method
vc	1.105	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.99	J/molxK	783.46	Joback Method
cpg	923.12	J/molxK	814.19	Joback Method
cpg	940.29	J/molxK	844.93	Joback Method
cpg	956.54	J/molxK	875.66	Joback Method
cpg	971.91	J/molxK	906.39	Joback Method
cpg	986.46	J/molxK	937.12	Joback Method
cpg	1000.23	J/molxK	967.86	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=U321196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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