

Sarcosine, N-cyclopropylcarbonyl-, hexadecyl ester

Inchi:	InChI=1S/C23H43NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-27-22(25)20-24(2)23(
InchiKey:	KWHWNHQXEQEZTP-UHFFFAOYSA-N
Formula:	C23H43NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C1CC1
Mol. weight [g/mol]:	381.59

Physical Properties

Property code	Value	Unit	Source
gf	-48.53	kJ/mol	Joback Method
hf	-735.10	kJ/mol	Joback Method
hfus	60.87	kJ/mol	Joback Method
hvap	84.65	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.879		Crippen Method
mcvol	343.060	ml/mol	McGowan Method
pc	983.31	kPa	Joback Method
rinpola	2929.00		NIST Webbook
tb	874.98	K	Joback Method
tc	1071.35	K	Joback Method
tf	521.47	K	Joback Method
vc	1.329	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1150.34	J/molxK	874.98	Joback Method
cpg	1170.16	J/molxK	907.71	Joback Method
cpg	1188.85	J/molxK	940.44	Joback Method
cpg	1206.50	J/molxK	973.17	Joback Method
cpg	1223.16	J/molxK	1005.89	Joback Method
cpg	1238.90	J/molxK	1038.62	Joback Method
cpg	1253.80	J/molxK	1071.35	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=U321199&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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