

Sarcosine, N-cyclopropylcarbonyl-, heptadecyl ester

Inchi: InChI=1S/C24H45NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-28-23(26)21-25(2)
InchiKey: VEQOREKLTDPSGH-UHFFFAOYSA-N
Formula: C24H45NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C1CC1
Mol. weight [g/mol]: 395.62

Physical Properties

Property code	Value	Unit	Source
gf	-40.11	kJ/mol	Joback Method
hf	-755.74	kJ/mol	Joback Method
hfus	63.46	kJ/mol	Joback Method
hvap	86.88	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	6.269		Crippen Method
mcvol	357.150	ml/mol	McGowan Method
pc	926.68	kPa	Joback Method
rinpol	3087.00		NIST Webbook
tb	897.86	K	Joback Method
tc	1099.34	K	Joback Method
tf	532.74	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.46	J/mol×K	897.86	Joback Method
cpg	1233.82	J/mol×K	931.44	Joback Method
cpg	1253.00	J/mol×K	965.02	Joback Method
cpg	1271.09	J/mol×K	998.60	Joback Method
cpg	1288.15	J/mol×K	1032.18	Joback Method
cpg	1304.27	J/mol×K	1065.76	Joback Method
cpg	1319.52	J/mol×K	1099.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321200&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
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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