Sarcosine, N-cyclopropylcarbonyl-, hexyl ester

Inchi: InChI=1S/C13H23NO3/c1-3-4-5-6-9-17-12(15)10-14(2)13(16)11-7-8-11/h11H,3-10H2,1-2

InchiKey: LOQHHSSIKMOENL-UHFFFAOYSA-N

Formula: C13H23NO3

SMILES: CCCCCCOC(=O)CN(C)C(=O)C1CC1

Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
gf	-132.73	kJ/mol	Joback Method
hf	-528.70	kJ/mol	Joback Method
hfus	34.97	kJ/mol	Joback Method
hvap	62.39	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.978		Crippen Method
mcvol	202.160	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	1851.00		NIST Webbook
tb	646.18	K	Joback Method
tc	831.41	K	Joback Method
tf	408.77	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.00	J/mol×K	646.18	Joback Method
cpg	581.01	J/mol×K	677.05	Joback Method
cpg	596.16	J/mol×K	707.92	Joback Method
cpg	610.50	J/mol×K	738.80	Joback Method
cpg	624.06	J/mol×K	769.67	Joback Method
cpg	636.88	J/mol×K	800.54	Joback Method
cpg	649.00	J/mol×K	831.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321191&Units=SI

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