Sarcosine, N-cyclopropylcarbonyl-, isohexyl ester

Inchi: InChI=1S/C13H23NO3/c1-10(2)5-4-8-17-12(15)9-14(3)13(16)11-6-7-11/h10-11H,4-9H2,1

InchiKey: LUMNSPBBMANNPI-UHFFFAOYSA-N

Formula: C13H23NO3

SMILES: CC(C)CCCOC(=O)CN(C)C(=O)C1CC1

Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
gf	-135.17	kJ/mol	Joback Method
hf	-533.98	kJ/mol	Joback Method
hfus	31.45	kJ/mol	Joback Method
hvap	62.00	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.834		Crippen Method
mcvol	202.160	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1805.00		NIST Webbook
rinpol	1805.00		NIST Webbook
tb	645.74	K	Joback Method
tc	834.02	K	Joback Method
tf	393.77	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.44	J/mol×K	645.74	Joback Method
cpg	581.75	J/mol×K	677.12	Joback Method
cpg	597.17	J/mol×K	708.50	Joback Method
cpg	611.74	J/mol×K	739.88	Joback Method
cpg	625.49	J/mol×K	771.26	Joback Method
cpg	638.48	J/mol×K	802.64	Joback Method
cpg	650.73	J/mol×K	834.02	Joback Method

Sources

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=U321190&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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