Sarcosine, N-(cyclohexylcarbonyl)-, propyl ester

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

InchiKey: JIBHYYAKGHVNNO-UHFFFAOYSA-N

Formula: C13H23NO3

SMILES: CCCOC(=O)CN(C)C(=O)C1CCCCC1

Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
gf	-169.03	kJ/mol	Joback Method
hf	-547.18	kJ/mol	Joback Method
hfus	28.67	kJ/mol	Joback Method
hvap	62.91	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.978		Crippen Method
mcvol	202.160	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1854.00		NIST Webbook
rinpol	1854.00		NIST Webbook
tb	658.99	K	Joback Method
tc	860.45	K	Joback Method
tf	398.21	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.19	J/mol×K	658.99	Joback Method
cpg	590.39	J/mol×K	692.57	Joback Method
cpg	607.50	J/mol×K	726.14	Joback Method
cpg	623.54	J/mol×K	759.72	Joback Method
cpg	638.55	J/mol×K	793.30	Joback Method
cpg	652.54	J/mol×K	826.87	Joback Method
cpg	665.55	J/mol×K	860.45	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=U321529&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