Sarcosine, N-(cyclohexylcarbonyl)-, butyl ester

Inchi: InChI=1S/C14H25NO3/c1-3-4-10-18-13(16)11-15(2)14(17)12-8-6-5-7-9-12/h12H,3-11H2

InchiKey: GWCPHHFWKCSNBT-UHFFFAOYSA-N

Formula: C14H25NO3

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

Mol. weight [g/mol]: 255.35

Physical Properties

Property code	Value	Unit	Source
gf	-160.61	kJ/mol	Joback Method
hf	-567.82	kJ/mol	Joback Method
hfus	31.26	kJ/mol	Joback Method
hvap	65.13	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.368		Crippen Method
mcvol	216.250	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
tb	681.87	K	Joback Method
tc	880.92	K	Joback Method
tf	409.48	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.06	J/mol×K	681.87	Joback Method
cpg	645.52	J/mol×K	715.05	Joback Method
cpg	662.87	J/mol×K	748.22	Joback Method
cpg	679.13	J/mol×K	781.40	Joback Method
cpg	694.34	J/mol×K	814.57	Joback Method
cpg	708.53	J/mol×K	847.75	Joback Method
cpg	721.71	J/mol×K	880.92	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=U321530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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