

Sarcosine, N-cyclopropylcarbonyl-, butyl ester

Inchi:	InChI=1S/C11H19NO3/c1-3-4-7-15-10(13)8-12(2)11(14)9-5-6-9/h9H,3-8H2,1-2H3
InchiKey:	WQTOMRSEBYPBMK-UHFFFAOYSA-N
Formula:	C11H19NO3
SMILES:	CCCCOC(=O)CN(C)C(=O)C1CC1
Mol. weight [g/mol]:	213.27

Physical Properties

Property code	Value	Unit	Source
gf	-149.57	kJ/mol	Joback Method
hf	-487.42	kJ/mol	Joback Method
hfus	29.79	kJ/mol	Joback Method
hvap	57.94	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.198		Crippen Method
mvol	173.980	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
tb	600.42	K	Joback Method
tc	789.27	K	Joback Method
tf	386.23	K	Joback Method
vc	0.656	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.44	J/molxK	600.42	Joback Method
cpg	476.50	J/molxK	631.89	Joback Method
cpg	490.73	J/molxK	663.37	Joback Method
cpg	504.19	J/molxK	694.84	Joback Method
cpg	516.90	J/molxK	726.32	Joback Method
cpg	528.89	J/molxK	757.79	Joback Method
cpg	540.22	J/molxK	789.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321188&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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