Sarcosine, N-cyclopropylcarbonyl-, ethyl ester

Inchi: InChI=1S/C9H15NO3/c1-3-13-8(11)6-10(2)9(12)7-4-5-7/h7H,3-6H2,1-2H3
InchiKey: DNWRLRKXQUEFES-UHFFFAOYSA-N
Formula: C9H15NO3
SMILES: CCOC(=O)CN(C)C(=O)C1CC1
Mol. weight [g/mol]: 185.22

Physical Properties

Property code	Value	Unit	Source
gf	-166.41	kJ/mol	Joback Method
hf	-446.14	kJ/mol	Joback Method
hfus	24.61	kJ/mol	Joback Method
hvap	53.49	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	0.418		Crippen Method
mcvol	145.800	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
tb	554.66	K	Joback Method
tc	748.12	K	Joback Method
tf	363.69	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.88	J/mol×K	554.66	Joback Method
cpg	377.69	J/mol×K	586.90	Joback Method
cpg	390.74	J/mol×K	619.15	Joback Method
cpg	403.05	J/mol×K	651.39	Joback Method
cpg	414.65	J/mol×K	683.64	Joback Method
cpg	425.59	J/mol×K	715.88	Joback Method
cpg	435.89	J/mol×K	748.12	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=U321186&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