

Sarcosine, N-cyclopropylcarbonyl-, propyl ester

Inchi:	InChI=1S/C10H17NO3/c1-3-6-14-9(12)7-11(2)10(13)8-4-5-8/h8H,3-7H2,1-2H3
InchiKey:	GPZMXAODLGGDCC-UHFFFAOYSA-N
Formula:	C10H17NO3
SMILES:	CCCOC(=O)CN(C)C(=O)C1CC1
Mol. weight [g/mol]:	199.25

Physical Properties

Property code	Value	Unit	Source
gf	-157.99	kJ/mol	Joback Method
hf	-466.78	kJ/mol	Joback Method
hfus	27.20	kJ/mol	Joback Method
hvap	55.71	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	0.808		Crippen Method
mcvol	159.890	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1554.00		NIST Webbook
rinpol	1554.00		NIST Webbook
tb	577.54	K	Joback Method
tc	768.59	K	Joback Method
tf	374.96	K	Joback Method
vc	0.601	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.87	J/mol×K	577.54	Joback Method
cpg	426.34	J/mol×K	609.38	Joback Method
cpg	440.02	J/mol×K	641.22	Joback Method
cpg	452.94	J/mol×K	673.07	Joback Method
cpg	465.14	J/mol×K	704.91	Joback Method
cpg	476.64	J/mol×K	736.75	Joback Method
cpg	487.48	J/mol×K	768.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321187&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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