

Sarcosine, N-cyclopropylcarbonyl-, heptyl ester

Inchi:	InChI=1S/C14H25NO3/c1-3-4-5-6-7-10-18-13(16)11-15(2)14(17)12-8-9-12/h12H,3-11H2
InchiKey:	RJHZLDVRQVLVTR-UHFFFAOYSA-N
Formula:	C14H25NO3
SMILES:	CCCCCCCOC(=O)CN(C)C(=O)C1CC1
Mol. weight [g/mol]:	255.35

Physical Properties

Property code	Value	Unit	Source
gf	-124.31	kJ/mol	Joback Method
hf	-549.34	kJ/mol	Joback Method
hfus	37.56	kJ/mol	Joback Method
hvap	64.62	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.368		Crippen Method
mcvol	216.250	ml/mol	McGowan Method
pc	1849.92	kPa	Joback Method
rinqol	1957.00		NIST Webbook
tb	669.06	K	Joback Method
tc	852.99	K	Joback Method
tf	420.04	K	Joback Method
vc	0.825	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.81	J/molxK	669.06	Joback Method
cpg	635.22	J/molxK	699.72	Joback Method
cpg	650.76	J/molxK	730.37	Joback Method
cpg	665.47	J/molxK	761.03	Joback Method
cpg	679.39	J/molxK	791.68	Joback Method
cpg	692.55	J/molxK	822.34	Joback Method
cpg	704.99	J/molxK	852.99	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=U321192&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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