Sarcosine, N-cyclopropylcarbonyl-, pentyl ester

Inchi: InChI=1S/C12H21NO3/c1-3-4-5-8-16-11(14)9-13(2)12(15)10-6-7-10/h10H,3-9H2,1-2H3
InchiKey: GLNAXEIENUMHCR-UHFFFAOYSA-N
Formula: C12H21NO3
SMILES: CCCCCOC(=O)CN(C)C(=O)C1CC1
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
gf	-141.15	kJ/mol	Joback Method
hf	-508.06	kJ/mol	Joback Method
hfus	32.38	kJ/mol	Joback Method
hvap	60.16	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.588		Crippen Method
mcvol	188.070	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1748.00		NIST Webbook
tb	623.30	K	Joback Method
tc	810.19	K	Joback Method
tf	397.50	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.52	J/mol×K	623.30	Joback Method
cpg	528.08	J/mol×K	654.45	Joback Method
cpg	542.80	J/mol×K	685.60	Joback Method
cpg	556.72	J/mol×K	716.74	Joback Method
cpg	569.89	J/mol×K	747.89	Joback Method
cpg	582.32	J/mol×K	779.04	Joback Method
cpg	594.06	J/mol×K	810.19	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=U321189&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