Sarcosine, N-(cyclopentylcarbonyl)-, pentyl ester

Inchi: InChI=1S/C14H25NO3/c1-3-4-7-10-18-13(16)11-15(2)14(17)12-8-5-6-9-12/h12H,3-11H2

InchiKey: SLRKPOSWRZCCEY-UHFFFAOYSA-N

Formula: C14H25NO3

SMILES: CCCCCOC(=O)CN(C)C(=O)C1CCCC1

Mol. weight [g/mol]: 255.35

Physical Properties

Property code	Value	Unit	Source
gf	-148.51	kJ/mol	Joback Method
hf	-561.66	kJ/mol	Joback Method
hfus	33.36	kJ/mol	Joback Method
hvap	64.96	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.368		Crippen Method
mcvol	216.250	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
tb	677.60	K	Joback Method
tc	871.35	K	Joback Method
tf	413.00	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.23	J/mol×K	677.60	Joback Method
cpg	641.98	J/mol×K	709.89	Joback Method
cpg	658.70	J/mol×K	742.18	Joback Method
cpg	674.44	J/mol×K	774.48	Joback Method
cpg	689.22	J/mol×K	806.77	Joback Method
cpg	703.08	J/mol×K	839.06	Joback Method
cpg	716.04	J/mol×K	871.35	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=U321337&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