Sarcosine, N-(cyclohexylcarbonyl)-, pentyl ester

Inchi: InChI=1S/C15H27NO3/c1-3-4-8-11-19-14(17)12-16(2)15(18)13-9-6-5-7-10-13/h13H,3-12
InchiKey: HAOTZMHTWYKLPU-UHFFFAOYSA-N
Formula: C15H27NO3
SMILES: CCCCCOC(=O)CN(C)C(=O)C1CCCCC1
Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
gf	-152.19	kJ/mol	Joback Method
hf	-588.46	kJ/mol	Joback Method
hfus	33.85	kJ/mol	Joback Method
hvap	67.36	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.758		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	2054.00		NIST Webbook
tb	704.75	K	Joback Method
tc	901.79	K	Joback Method
tf	420.75	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.10	J/mol×K	704.75	Joback Method
cpg	701.77	J/mol×K	737.59	Joback Method
cpg	719.31	J/mol×K	770.43	Joback Method
cpg	735.75	J/mol×K	803.27	Joback Method
cpg	751.11	J/mol×K	836.11	Joback Method
cpg	765.44	J/mol×K	868.95	Joback Method
cpg	778.75	J/mol×K	901.79	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=U321531&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

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