Sarcosine, N-(3-cyclopentylpropionyl)-, pentyl ester

Inchi: InChI=1S/C16H29NO3/c1-3-4-7-12-20-16(19)13-17(2)15(18)11-10-14-8-5-6-9-14/h14H,3

InchiKey: VKWHFIKDDUHTBA-UHFFFAOYSA-N

Formula: C16H29NO3

SMILES: CCCCCOC(=O)CN(C)C(=O)CCC1CCCC1

Mol. weight [g/mol]: 283.41

Physical Properties

Property code	Value	Unit	Source
gf	-131.67	kJ/mol	Joback Method
hf	-602.94	kJ/mol	Joback Method
hfus	38.54	kJ/mol	Joback Method
hvap	69.41	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.149		Crippen Method
mcvol	244.430	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	2179.00		NIST Webbook
rinpol	2179.00		NIST Webbook
tb	723.36	K	Joback Method
tc	914.29	K	Joback Method
tf	435.54	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.77	J/mol×K	723.36	Joback Method
cpg	755.02	J/mol×K	755.18	Joback Method
cpg	772.21	J/mol×K	787.00	Joback Method
cpg	788.38	J/mol×K	818.82	Joback Method
cpg	803.56	J/mol×K	850.64	Joback Method
cpg	817.78	J/mol×K	882.47	Joback Method
cpg	831.09	J/mol×K	914.29	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=U321833&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