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

Inchi: InChI=1S/C17H31NO3/c1-14(2)7-6-12-21-17(20)13-18(3)16(19)11-10-15-8-4-5-9-15/h14

InchiKey: BMTULLVCUJCXLS-UHFFFAOYSA-N

Formula: C17H31NO3

SMILES: CC(C)CCCOC(=O)CN(C)C(=O)CCC1CCCC1

Mol. weight [g/mol]: 297.43

Physical Properties

Property code	Value	Unit	Source
gf	-125.69	kJ/mol	Joback Method
hf	-628.86	kJ/mol	Joback Method
hfus	37.60	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.395		Crippen Method
mcvol	258.520	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	745.80	K	Joback Method
tc	938.40	K	Joback Method
tf	431.81	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.12	J/mol×K	745.80	Joback Method
cpg	813.83	J/mol×K	777.90	Joback Method
cpg	831.42	J/mol×K	810.00	Joback Method
cpg	847.94	J/mol×K	842.10	Joback Method
cpg	863.41	J/mol×K	874.20	Joback Method
cpg	877.89	J/mol×K	906.30	Joback Method
cpg	891.40	J/mol×K	938.40	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=U321834&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