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

Inchi: InChI=1S/C15H27NO3/c1-12(2)11-19-15(18)10-16(3)14(17)9-8-13-6-4-5-7-13/h12-13H,4

InchiKey: CGTCBOUATQPIAS-UHFFFAOYSA-N

Formula: C15H27NO3

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

Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
gf	-142.53	kJ/mol	Joback Method
hf	-587.58	kJ/mol	Joback Method
hfus	32.42	kJ/mol	Joback Method
hvap	66.80	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.614		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	2044.00		NIST Webbook
tb	700.04	K	Joback Method
tc	895.08	K	Joback Method
tf	409.27	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.41	J/mol×K	700.04	Joback Method
cpg	698.73	J/mol×K	732.55	Joback Method
cpg	715.96	J/mol×K	765.05	Joback Method
cpg	732.15	J/mol×K	797.56	Joback Method
cpg	747.32	J/mol×K	830.07	Joback Method
cpg	761.53	J/mol×K	862.57	Joback Method
cpg	774.79	J/mol×K	895.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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