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

Inchi: InChI=1S/C15H27NO3/c1-3-4-11-19-15(18)12-16(2)14(17)10-9-13-7-5-6-8-13/h13H,3-12

InchiKey: QILYZJOTHHUBBY-UHFFFAOYSA-N

Formula: C15H27NO3

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

Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
gf	-140.09	kJ/mol	Joback Method
hf	-582.30	kJ/mol	Joback Method
hfus	35.95	kJ/mol	Joback Method
hvap	67.19	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.758		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	2091.00		NIST Webbook
tb	700.48	K	Joback Method
tc	892.60	K	Joback Method
tf	424.27	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.94	J/mol×K	700.48	Joback Method
cpg	697.96	J/mol×K	732.50	Joback Method
cpg	714.94	J/mol×K	764.52	Joback Method
cpg	730.90	J/mol×K	796.54	Joback Method
cpg	745.90	J/mol×K	828.56	Joback Method
cpg	759.96	J/mol×K	860.58	Joback Method
cpg	773.11	J/mol×K	892.60	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=U321832&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