«beta»-Alanine, N-(3-cyclopentylpropionyl)-, butyl ester

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

InchiKey: AZFKGAUNZXZOSJ-UHFFFAOYSA-N

Formula: C15H27NO3

SMILES: CCCCOC(=O)CCNC(=O)CCC1CCCC1

Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
gf	-161.48	kJ/mol	Joback Method
hf	-596.36	kJ/mol	Joback Method
hfus	38.03	kJ/mol	Joback Method
hvap	71.58	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.806		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	2149.00		NIST Webbook
tb	738.21	K	Joback Method
tc	933.63	K	Joback Method
tf	444.46	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.37	J/mol×K	738.21	Joback Method
cpg	716.54	J/mol×K	770.78	Joback Method
cpg	732.68	J/mol×K	803.35	Joback Method
cpg	747.81	J/mol×K	835.92	Joback Method
cpg	761.98	J/mol×K	868.49	Joback Method
cpg	775.20	J/mol×K	901.06	Joback Method
cpg	787.52	J/mol×K	933.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321752&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

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