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

Inchi: InChI=1S/C13H23NO3/c1-2-17-13(16)9-10-14-12(15)8-7-11-5-3-4-6-11/h11H,2-10H2,1H

InchiKey: BKSMZXSKVQDARR-UHFFFAOYSA-N

Formula: C13H23NO3

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

Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
gf	-178.32	kJ/mol	Joback Method
hf	-555.08	kJ/mol	Joback Method
hfus	32.85	kJ/mol	Joback Method
hvap	67.13	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.026		Crippen Method
mcvol	202.160	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1943.00		NIST Webbook
rinpol	1943.00		NIST Webbook
tb	692.45	K	Joback Method
tc	891.13	K	Joback Method
tf	421.92	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.97	J/mol×K	692.45	Joback Method
cpg	604.57	J/mol×K	725.56	Joback Method
cpg	620.18	J/mol×K	758.68	Joback Method
cpg	634.84	J/mol×K	791.79	Joback Method
cpg	648.57	J/mol×K	824.90	Joback Method
cpg	661.39	J/mol×K	858.02	Joback Method
cpg	673.33	J/mol×K	891.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321750&Units=SI

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