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

Inchi: InChI=1S/C14H25NO3/c1-2-11-18-14(17)9-10-15-13(16)8-7-12-5-3-4-6-12/h12H,2-11H2

InchiKey: HHPRPBZOMRULFD-UHFFFAOYSA-N

Formula: C14H25NO3

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

Mol. weight [g/mol]: 255.35

Physical Properties

Property code	Value	Unit	Source
gf	-169.90	kJ/mol	Joback Method
hf	-575.72	kJ/mol	Joback Method
hfus	35.44	kJ/mol	Joback Method
hvap	69.35	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.416		Crippen Method
mcvol	216.250	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	2048.00		NIST Webbook
rinpol	2048.00		NIST Webbook
tb	715.33	K	Joback Method
tc	912.15	K	Joback Method
tf	433.19	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.11	J/mol×K	715.33	Joback Method
cpg	660.01	J/mol×K	748.13	Joback Method
cpg	675.91	J/mol×K	780.94	Joback Method
cpg	690.83	J/mol×K	813.74	Joback Method
cpg	704.79	J/mol×K	846.54	Joback Method
cpg	717.84	J/mol×K	879.34	Joback Method
cpg	729.98	J/mol×K	912.15	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=U321751&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