«beta»-Alanine, N-cyclohexylcarbonyl-, propyl ester

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

InchiKey: GHQRLSXSUSRJEH-UHFFFAOYSA-N

Formula: C13H23NO3

SMILES: CCCOC(=O)CCNC(=O)C1CCCCC1

Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
gf	-190.42	kJ/mol	Joback Method
hf	-561.24	kJ/mol	Joback Method
hfus	30.75	kJ/mol	Joback Method
hvap	67.30	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.026		Crippen Method
mcvol	202.160	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook
tb	696.72	K	Joback Method
tc	900.83	K	Joback Method
tf	418.40	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.77	J/mol×K	696.72	Joback Method
cpg	608.05	J/mol×K	730.74	Joback Method
cpg	624.25	J/mol×K	764.76	Joback Method
cpg	639.39	J/mol×K	798.78	Joback Method
cpg	653.50	J/mol×K	832.80	Joback Method
cpg	666.59	J/mol×K	866.81	Joback Method
cpg	678.70	J/mol×K	900.83	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=U321961&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