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

Inchi: InChI=1S/C12H21NO3/c1-2-16-11(14)8-9-13-12(15)10-6-4-3-5-7-10/h10H,2-9H2,1H3,(H

InchiKey: YPTRFXLVRQUQMC-UHFFFAOYSA-N

Formula: C12H21NO3

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

Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
gf	-198.84	kJ/mol	Joback Method
hf	-540.60	kJ/mol	Joback Method
hfus	28.16	kJ/mol	Joback Method
hvap	65.07	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.636		Crippen Method
mcvol	188.070	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1826.00		NIST Webbook
tb	673.84	K	Joback Method
tc	880.62	K	Joback Method
tf	407.13	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.48	J/mol×K	673.84	Joback Method
cpg	553.46	J/mol×K	708.30	Joback Method
cpg	569.38	J/mol×K	742.77	Joback Method
cpg	584.27	J/mol×K	777.23	Joback Method
cpg	598.14	J/mol×K	811.69	Joback Method
cpg	611.03	J/mol×K	846.16	Joback Method
cpg	622.93	J/mol×K	880.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321960&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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