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

Inchi: InChI=1S/C17H31NO3/c1-2-3-4-5-9-14-21-16(19)12-13-18-17(20)15-10-7-6-8-11-15/h15

InchiKey: UHAJWAQPTYMHMF-UHFFFAOYSA-N

Formula: C17H31NO3

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

Mol. weight [g/mol]: 297.43

Physical Properties

Property code	Value	Unit	Source
gf	-156.74	kJ/mol	Joback Method
hf	-643.80	kJ/mol	Joback Method
hfus	41.11	kJ/mol	Joback Method
hvap	76.20	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.587		Crippen Method
mcvol	258.520	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2349.00		NIST Webbook
tb	788.24	K	Joback Method
tc	986.29	K	Joback Method
tf	463.48	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.82	J/mol×K	788.24	Joback Method
cpg	836.87	J/mol×K	821.25	Joback Method
cpg	853.74	J/mol×K	854.26	Joback Method
cpg	869.46	J/mol×K	887.27	Joback Method
cpg	884.05	J/mol×K	920.27	Joback Method
cpg	897.56	J/mol×K	953.28	Joback Method
cpg	910.01	J/mol×K	986.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321964&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