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

Inchi: InChI=1S/C16H29NO3/c1-2-3-4-8-13-20-15(18)11-12-17-16(19)14-9-6-5-7-10-14/h14H,2

InchiKey: SDIMTASARFSZJH-UHFFFAOYSA-N

Formula: C16H29NO3

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

Mol. weight [g/mol]: 283.41

Physical Properties

Property code	Value	Unit	Source
gf	-165.16	kJ/mol	Joback Method
hf	-623.16	kJ/mol	Joback Method
hfus	38.52	kJ/mol	Joback Method
hvap	73.98	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.196		Crippen Method
mcvol	244.430	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	765.36	K	Joback Method
tc	964.14	K	Joback Method
tf	452.21	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.33	J/mol×K	765.36	Joback Method
cpg	778.23	J/mol×K	798.49	Joback Method
cpg	794.98	J/mol×K	831.62	Joback Method
cpg	810.60	J/mol×K	864.75	Joback Method
cpg	825.13	J/mol×K	897.88	Joback Method
cpg	838.58	J/mol×K	931.01	Joback Method
cpg	850.99	J/mol×K	964.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321963&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