1-Aminocyclopentanecarboxylic acid, N-hexyloxycarbonyl-, pentyl ester

Inchi: InChI=1S/C18H33NO4/c1-3-5-7-11-15-23-17(21)19-18(12-8-9-13-18)16(20)22-14-10-6-4

InchiKey: KLOGLQPPRYBXGS-UHFFFAOYSA-N

Formula: C18H33NO4

SMILES: CCCCCCOC(O)=NC1(C(=O)OCCCCC)CCCC1

Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
hf	-795.95	kJ/mol	Joback Method
hvap	86.41	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.544		Crippen Method
mcvol	278.480	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	2257.00		NIST Webbook
rinpol	2257.00		NIST Webbook
tb	894.21	K	Joback Method
tc	1099.15	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392427&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

Legend

hf: Enthalpy of formation 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