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

Inchi: InChI=1S/C22H41NO4/c1-3-5-7-9-10-11-15-18-26-20(24)22(16-12-13-17-22)23-21(25)27

InchiKey: IXVCTPGJZQTWPU-UHFFFAOYSA-N

Formula: C22H41NO4

SMILES: CCCCCCCCCOC(=O)C1(N=C(O)OCCCCCC)CCCC1

Mol. weight [g/mol]: 383.57

Physical Properties

Property code	Value	Unit	Source
hf	-878.51	kJ/mol	Joback Method
hvap	95.31	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	6.104		Crippen Method
mcvol	334.840	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	2652.00		NIST Webbook
rinpol	2652.00		NIST Webbook
tb	985.73	K	Joback Method
tc	1207.32	K	Joback Method

Sources

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=U392431&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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