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

Inchi: InChI=1S/C21H39NO4/c1-3-5-7-9-10-14-17-25-19(23)21(15-11-12-16-21)22-20(24)26-18

InchiKey: SGJKHONPESDQHY-UHFFFAOYSA-N

Formula: C21H39NO4

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

Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
hf	-857.87	kJ/mol	Joback Method
hvap	93.08	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.714		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2550.00		NIST Webbook
rinpol	2550.00		NIST Webbook
tb	962.85	K	Joback Method
tc	1178.80	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392430&Units=SI

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

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