1-Aminocyclopentanecarboxylic acid, N-(octyloxycarbonyl)-, decyl ester

Inchi: InChI=1S/C25H47NO4/c1-3-5-7-9-11-12-14-17-21-29-23(27)25(19-15-16-20-25)26-24(28

InchiKey: JRIUCUMQMGNLIO-UHFFFAOYSA-N

Formula: C25H47NO4

SMILES: CCCCCCCCCCOC(=O)C1(N=C(O)OCCCCCCCC)CCCC1

Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
hf	-940.43	kJ/mol	Joback Method
hvap	101.99	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	7.274		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
pc	879.48	kPa	Joback Method
rinpol	2846.00		NIST Webbook
rinpol	2846.00		NIST Webbook
tb	1054.37	K	Joback Method
tc	1299.84	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392566&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

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