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

Inchi: InChI=1S/C23H43NO4/c1-3-5-7-9-11-15-19-27-21(25)23(17-13-14-18-23)24-22(26)28-20

InchiKey: KMMNFVQQUNOOGH-UHFFFAOYSA-N

Formula: C23H43NO4

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

Mol. weight [g/mol]: 397.59

Physical Properties

Property code	Value	Unit	Source
hf	-899.15	kJ/mol	Joback Method
hvap	97.54	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.494		Crippen Method
mcvol	348.930	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	2660.00		NIST Webbook
rinpol	2660.00		NIST Webbook
tb	1008.61	K	Joback Method
tc	1236.94	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392564&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

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