1-Aminocyclopentanecarboxylic acid, N-(benzyloxycarbonyl)-, pentyl ester

Inchi: InChI=1S/C19H27NO4/c1-2-3-9-14-23-17(21)19(12-7-8-13-19)20-18(22)24-15-16-10-5-4

InchiKey: RZHJUWSCYZKDBS-UHFFFAOYSA-N

Formula: C19H27NO4

SMILES: CCCCCOC(=O)C1(N=C(O)OCc2ccccc2)CCCC1

Mol. weight [g/mol]: 333.42

Physical Properties

Property code	Value	Unit	Source
hf	-580.06	kJ/mol	Joback Method
hvap	90.91	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.163		Crippen Method
mcvol	268.810	ml/mol	McGowan Method
pc	1645.76	kPa	Joback Method
rinpol	2473.00		NIST Webbook
rinpol	2473.00		NIST Webbook
tb	943.77	K	Joback Method
tc	1167.41	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392529&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