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

Inchi: InChI=1S/C21H31NO4/c1-2-3-4-5-11-16-25-19(23)21(14-9-10-15-21)22-20(24)26-17-18-

InchiKey: MVWADUBESNPWLE-UHFFFAOYSA-N

Formula: C21H31NO4

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

Mol. weight [g/mol]: 361.48

Physical Properties

Property code	Value	Unit	Source
hf	-621.34	kJ/mol	Joback Method
hvap	95.36	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.944		Crippen Method
mcvol	296.990	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook
tb	989.53	K	Joback Method
tc	1215.75	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392530&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