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

Inchi: InChI=1S/C21H23NO4/c23-19(25-15-17-9-3-1-4-10-17)21(13-7-8-14-21)22-20(24)26-16-
InchiKey: YJNOHNQHJVAPTD-UHFFFAOYSA-N
Formula: C21H23NO4
SMILES: O=C(OCc1ccccc1)C1(N=C(O)OCc2ccccc2)CCCC1
Mol. weight [g/mol]: 353.41

Physical Properties

Property code	Value	Unit	Source
hf	-384.81	kJ/mol	Joback Method
hvap	97.64	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.173		Crippen Method
mcvol	273.230	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	2850.00		NIST Webbook
rinpol	2850.00		NIST Webbook
tb	1016.21	K	Joback Method
tc	1261.81	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392531&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