

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

Inchi: InChI=1S/C18H25NO4/c1-2-3-13-22-16(20)18(11-7-8-12-18)19-17(21)23-14-15-9-5-4-6-
InchiKey: CXNBXRAWINAMNA-UHFFFAOYSA-N
Formula: C18H25NO4
SMILES: CCCOC(=O)C1(N=C(O)OCc2ccccc2)CCCC1
Mol. weight [g/mol]: 319.40

Physical Properties

Property code	Value	Unit	Source
hf	-559.42	kJ/mol	Joback Method
hvap	88.68	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.773		Crippen Method
mcvol	254.720	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
rinpol	2374.00		NIST Webbook
tb	920.89	K	Joback Method
tc	1144.51	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392528&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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