

5-Methoxytryptamine, iso-BOC

Inchi: InChI=1S/C21H30N2O5/c1-14(2)12-27-20(24)22-9-8-16-11-23(21(25)28-13-15(3)4)19-7
InchiKey: WUIMKJZEOJEOAW-UHFFFAOYSA-N
Formula: C21H30N2O5
SMILES: COc1ccc2c(c1)c(CCNC(=O)OCC(C)C)cn2C(=O)OCC(C)C
Mol. weight [g/mol]: 390.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.80		Crippen Method
logp	4.215		Crippen Method
mcvol	308.540	ml/mol	McGowan Method
rinpol	2616.00		NIST Webbook
rinpol	2616.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R499446&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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