Tryptamine, iso-BOC

Inchi: InChI=1S/C20H28N2O4/c1-14(2)12-25-19(23)21-10-9-16-11-22(20(24)26-13-15(3)4)18-8
InchiKey: XGHSMQXXJQCQNK-UHFFFAOYSA-N
Formula: C20H28N2O4
SMILES: CC(C)COC(=O)NCCc1cn(C(=O)OCC(C)C)c2ccccc12
Mol. weight [g/mol]: 360.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.68		Crippen Method
logp	4.207		Crippen Method
mcvol	288.580	ml/mol	McGowan Method
rinpol	2387.00		NIST Webbook
rinpol	2387.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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=R392875&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.