

3'-hydroxy-N-benzylpiperazine, diTFA

Inchi: InChI=1S/C15H14F6N2O3/c16-14(17,18)12(24)23-6-4-22(5-7-23)9-10-2-1-3-11(8-10)26-15
InchiKey: TXJMIQBSJGYMTN-UHFFFAOYSA-N
Formula: C15H14F6N2O3
SMILES: O=C(Oc1ccccc(CN2CCN(C(=O)C(F)(F)F)CC2)c1)C(F)(F)F
Mol. weight [g/mol]: 384.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	2.361		Crippen Method
mcvol	227.180	ml/mol	McGowan Method
rinpol	1889.00		NIST Webbook
rinpol	1889.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R418685&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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<https://www.chemeo.com/cid/26-378-4/3-hydroxy-N-benzylpiperazine-diTFA.pdf>

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