

4'-hydroxy-N-benzylpiperazine, diTFA

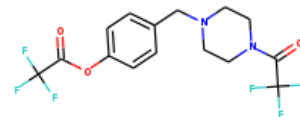
InChI: InChI=1S/C15H14F6N2O3/c16-14(17,18)12(24)23-7-5-22(6-8-23)
9-10-1-3-11(4-2-10)26-13(25)15(19,20)21/h1-4H,5-9H2

InChI Key: NEIMYVDHROEYAC-UHFFFAOYSA-N

Formula: C15H14F6N2O3

SMILES: O=C(Oc1ccc(CN2CCN(C(=O)C(F)(F)F)CC2)cc1)C(F)(F)F

Molecular Weight: 384.27



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	2.36		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H14F6N2O3/c16-14\(17,18\)12\(24\)23-7-5-22\(6-8-23\)9-10-1-3-11\(4-2-10\)26-13\(25\)15\(19,20\)21/h1-4H,5-9H2](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H14F6N2O3/c16-14(17,18)12(24)23-7-5-22(6-8-23)9-10-1-3-11(4-2-10)26-13(25)15(19,20)21/h1-4H,5-9H2)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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