

# 4'-hydroxy-N-benzylpiperazine, diTFA

<b>Inchi:</b>	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
<b>InchiKey:</b>	NEIMYVDHROEYAC-UHFFFAOYSA-N
<b>Formula:</b>	C15H14F6N2O3
<b>SMILES:</b>	O=C(Oc1ccc(CN2CCN(C(=O)C(F)(F)F)CC2)cc1)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	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	1847.00		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R418709&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R418709&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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