

# N-benzylpiperazine, TFA

**Inchi:** InChI=1S/C13H15F3N2O/c14-13(15,16)12(19)18-8-6-17(7-9-18)10-11-4-2-1-3-5-11/h1-5  
**InchiKey:** VZIHGMYACKUQQJ-UHFFFAOYSA-N  
**Formula:** C13H15F3N2O  
**SMILES:** O=C(N1CCN(Cc2ccccc2)CC1)C(F)(F)F  
**Mol. weight [g/mol]:** 272.27

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.33		Crippen Method
logp	1.893		Crippen Method
mcvol	186.250	ml/mol	McGowan Method
rinpol	1718.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R418714&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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