

# 1-(8-Bromo-dibenzo[1,2-b; 4,5-b']difuran-4-yl)-2-aminoethane, TFA

**Inchi:** InChI=1S/C14H9BrF3NO3/c15-10-9-3-6-21-11(9)7(8-2-5-22-12(8)10)1-4-19-13(20)14(16)  
**InchiKey:** XQPQIGFLPPMSGH-UHFFFAOYSA-N  
**Formula:** C14H9BrF3NO3  
**SMILES:** O=C(NCCc1c2ccoc2c(Br)c2ccoc12)C(F)(F)F  
**Mol. weight [g/mol]:** 376.12

## Physical Properties

Property code	Value	Unit	Source
log10ws	-14.98		Crippen Method
logp	4.163		Crippen Method
mcvol	200.140	ml/mol	McGowan Method
rinpol	2137.00		NIST Webbook
rinpol	2189.00		NIST Webbook
rinpol	2137.00		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=R640530&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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