# 1-(8-Bromo-2,3,6,7-tetrahydrodibenzo[1,2-b;4,5-b']difuran-4-yl-2-aminoethane, TFA

**Inchi:** InChI=1S/C14H13BrF3NO3/c15-10-9-3-6-21-11(9)7(8-2-5-22-12(8)10)1-4-19-13(20)14(1

**InchiKey:** LHOPHBFOOLNLLJ-UHFFFAOYSA-N

**Formula:** C14H13BrF3NO3

**SMILES:** OC(=NCCc1c2c(c(Br)c3c1OCC3)OCC2)C(F)(F)F

**Mol. weight [g/mol]:** 380.16

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -881.38 | kJ/mol | Joback Method |
| hvap | 84.57 | kJ/mol | Joback Method |
| log10ws | -4.72 | | Crippen Method |
| logp | 3.380 | | Crippen Method |
| mcvol | 208.740 | ml/mol | McGowan Method |
| pc | 2372.59 | kPa | Joback Method |
| rinpol | 2257.00 | | NIST Webbook |
| rinpol | 2309.00 | | NIST Webbook |
| rinpol | 2257.00 | | NIST Webbook |
| tb | 877.50 | K | Joback Method |
| tc | 1098.71 | K | Joback Method |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R640476&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

## Legend

**hf:** Enthalpy of formation at standard conditions

| | |
|---|---|
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |