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/ci990307l
Crippen Method: 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