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

Inchi: InChI=1S/C15H11BrF3NO3/c1-7(20-14(21)15(17,18)19)6-10-8-2-4-23-13(8)11(16)9-3-5-

InchiKey: PKXOSBKRNHIARG-UHFFFAOYSA-N

Formula: C15H11BrF3NO3

SMILES: CC(Cc1c2ccoc2c(Br)c2ccoc12)N=C(O)C(F)(F)F

Mol. weight [g/mol]: 390.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.53		Crippen Method
logp	5.391		Crippen Method
mcvol	214.230	ml/mol	McGowan Method
rinpol	2127.00		NIST Webbook
rinpol	2156.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R640570&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.