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

InChI: InChI=1S/C16H13BrF3NO3/c1-8(21(2)15(22)16(18,19)20)7-11-9-3-5-24-14(9)12(17)10-4

InchiKey: FJTMVPSFPRWJDV-UHFFFAOYSA-N

Formula: C16H13BrF3NO3

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

Mol. weight [g/mol]: 404.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.31		Crippen Method
logp	4.893		Crippen Method
mcvol	228.320	ml/mol	McGowan Method
rinpol	2230.00		NIST Webbook
rinpol	2274.00		NIST Webbook
rinpol	2230.00		NIST Webbook

Sources

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=R640565&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices