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

Inchi: InChI=1S/C12H10BrNO2/c13-10-9-3-6-15-11(9)7(1-4-14)8-2-5-16-12(8)10/h2-3,5-6H,1,4

InchiKey: JWBRIUSZWWDKGO-UHFFFAOYSA-N

Formula: C12H10BrNO2

SMILES: NCCc1c2ccoc2c(Br)c2ccoc12

Mol. weight [g/mol]: 280.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.95		Crippen Method
logp	3.443		Crippen Method
mcvol	165.080	ml/mol	McGowan Method
rinpol	2029.00		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=R640525&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