

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

Inchi: InChI=1S/C14H14BrNO2/c1-8(16-2)7-11-9-3-5-18-14(9)12(15)10-4-6-17-13(10)11/h3-6,8
InchiKey: YGBFIXUYJPFKTL-UHFFFAOYSA-N
Formula: C14H14BrNO2
SMILES: CNC(C)Cc1c2ccoc2c(Br)c2ccoc12
Mol. weight [g/mol]: 308.17

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -14.65 | | Crippen Method |
| logp | 4.092 | | Crippen Method |
| mcvol | 193.260 | ml/mol | McGowan Method |
| rinpol | 2081.00 | | NIST Webbook |
| rinpol | 2124.00 | | NIST Webbook |
| rinpol | 2081.00 | | 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=R640550&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/78-505-5/1-8-Bromo-dibenzo-1-2-b-4-5-b-difuran-4-yl-2-aminopropane-N-methyl.pdf>

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