

4-bromo-dibenzofuran

Inchi: InChI=1S/C12H7BrO/c13-10-6-3-5-9-8-4-1-2-7-11(8)14-12(9)10/h1-7H
InchiKey: DYT YBRPMNQFFL-UHFFFAOYSA-N
Formula: C₁₂H₇BrO
SMILES: Brc1cccc2c1oc1cccc12
Mol. weight [g/mol]: 247.09
CAS: 89827-45-2

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -9.98 | | Crippen Method |
| logp | 4.348 | | Crippen Method |
| mcvol | 144.930 | ml/mol | McGowan Method |
| rinpola | 1865.00 | | 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=C89827452&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
rinpola: Non-polar retention indices

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<https://www.chemeo.com/cid/93-913-5/4-bromo-dibenzofuran.pdf>

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