

4-Phenyldibenzofuran

Inchi: InChI=1S/C18H12O/c1-2-7-13(8-3-1)14-10-6-11-16-15-9-4-5-12-17(15)19-18(14)16/h1-11
InchiKey: JQIHNXZEJUGOSG-UHFFFAOYSA-N
Formula: C18H12O
SMILES: c1ccc(-c2cccc3c2oc2ccccc23)cc1
Mol. weight [g/mol]: 244.29

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -11.42 | | Crippen Method |
| logp | 5.253 | | Crippen Method |
| mcvol | 188.210 | ml/mol | McGowan Method |
| rinpol | 375.94 | | NIST Webbook |
| rinpol | 375.94 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U314395&Units=SI>

Legend

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

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