

4-Phenyldibenzothiophene

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|-----------------------------|--|
| Inchi: | InChI=1S/C18H12S/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: | BMCNAHBDZUYGJG-UHFFFAOYSA-N |
| Formula: | C18H12S |
| SMILES: | c1ccc(-c2cccc3c2sc2cccc23)cc1 |
| Mol. weight [g/mol]: | 260.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.44 | | Crippen Method |
| logp | 5.721 | | Crippen Method |
| mcvol | 198.690 | ml/mol | McGowan Method |
| rinpole | 405.68 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U314397&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

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

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