# 3-Phenyldibenzothiophene

**Inchi:** InChI=1S/C18H12S/c1-2-6-13(7-3-1)14-10-11-16-15-8-4-5-9-17(15)19-18(16)12-14/h1-1
**InchiKey:** SLQWXGMHQCRWHC-UHFFFAOYSA-N
**Formula:** C18H12S
**SMILES:** c1ccc(-c2ccc3c(c2)sc2ccccc23)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 |
| rinpol | 421.07 | | 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=R556480&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