# Dibenzothiophene, 1,8-dimethyl

**Other names:** 1,8-dimethyl-dibenzothiophene
**Inchi:** InChI=1S/C14H12S/c1-9-6-7-12-11(8-9)14-10(2)4-3-5-13(14)15-12/h3-8H,1-2H3
**InchiKey:** KMPJENUWHPZRGZ-UHFFFAOYSA-N
**Formula:** C14H12S
**SMILES:** Cc1ccc2sc3cccc(C)c3c2c1
**Mol. weight [g/mol]:** 212.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -5.79 | | Crippen Method |
| logp | 4.671 | | Crippen Method |
| mcvol | 166.090 | ml/mol | McGowan Method |
| rinpol | 335.65 | | NIST Webbook |
| rinpol | 332.86 | | NIST Webbook |
| rinpol | 332.86 | | NIST Webbook |
| rinpol | 335.65 | | 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=R67293&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