# 2,3,7,8-tetramethyl-dibenzothiophene

**Inchi:** InChI=1S/C16H16S/c1-9-5-13-14-6-10(2)12(4)8-16(14)17-15(13)7-11(9)3/h5-8H,1-4H3
**InchiKey:** KKFXTFLABPKUPX-UHFFFAOYSA-N
**Formula:** C16H16S
**SMILES:** Cc1cc2sc3cc(C)c(C)cc3c2cc1C
**Mol. weight [g/mol]:** 240.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -6.74 | | Crippen Method |
| logp | 5.288 | | Crippen Method |
| mcvol | 194.270 | ml/mol | McGowan Method |
| rinpol | 378.95 | | NIST Webbook |
| rinpol | 378.95 | | NIST Webbook |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R436103&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## 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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