# Dibenzothiophene, 3,6-dimethyl

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|---|---|
| **Other names:** | 3,6-dimethyl-dibenzothiophene |
| **Inchi:** | InChI=1S/C14H12S/c1-9-6-7-11-12-5-3-4-10(2)14(12)15-13(11)8-9/h3-8H,1-2H3 |
| **InchiKey:** | JTASASABTJTWTR-UHFFFAOYSA-N |
| **Formula:** | C14H12S |
| **SMILES:** | Cc1ccc2c(c1)sc1c(C)cccc12 |
| **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 | 331.49 | | NIST Webbook |
| rinpol | 333.44 | | NIST Webbook |
| rinpol | 332.80 | | NIST Webbook |
| rinpol | 333.40 | | NIST Webbook |
| rinpol | 332.90 | | NIST Webbook |
| rinpol | 332.90 | | NIST Webbook |
| rinpol | 332.88 | | NIST Webbook |
| rinpol | 329.25 | | NIST Webbook |
| rinpol | 332.88 | | NIST Webbook |

## Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R20964&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.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 |
| **rinpol:** | Non-polar retention indices |

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