

# 4,6-diethyl-dibenzothiophene

**Inchi:** InChI=1S/C16H16S/c1-3-11-7-5-9-13-14-10-6-8-12(4-2)16(14)17-15(11)13/h5-10H,3-4H2  
**InchiKey:** UMQGGSYHJPHWFV-UHFFFAOYSA-N  
**Formula:** C16H16S  
**SMILES:** CCc1cccc2c1sc1c(CC)cccc12  
**Mol. weight [g/mol]:** 240.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.44		Crippen Method
logp	5.179		Crippen Method
mcvol	194.270	ml/mol	McGowan Method
rinpol	352.57		NIST Webbook
rinpol	352.57		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R436232&Units=SI>

## 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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