

# 3-Ethyldibenzothiophene

**Inchi:** InChI=1S/C14H12S/c1-2-10-7-8-12-11-5-3-4-6-13(11)15-14(12)9-10/h3-9H,2H2,1H3  
**InchiKey:** WHCTVWMWBFBJKN-UHFFFAOYSA-N  
**Formula:** C14H12S  
**SMILES:** CCc1ccc2c(c1)sc1cccc12  
**Mol. weight [g/mol]:** 212.31  
**CAS:** 89817-03-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	4.617		Crippen Method
mccvol	166.090	ml/mol	McGowan Method
rinpol	328.17		NIST Webbook
rinpol	328.80		NIST Webbook
rinpol	328.50		NIST Webbook
rinpol	328.34		NIST Webbook
rinpol	329.77		NIST Webbook
rinpol	328.30		NIST Webbook
rinpol	328.50		NIST Webbook
rinpol	328.17		NIST Webbook
rinpol	329.77		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C89817038&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcpol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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