

# Benzo[b]phenanthro[3,2-d]thiophene

**Inchi:** InChI=1S/C20H12S/c1-2-6-15-13(5-1)9-10-14-11-20-18(12-17(14)15)16-7-3-4-8-19(16)2  
**InchiKey:** KBDUMZXQRUCDSI-UHFFFAOYSA-N  
**Formula:** C20H12S  
**SMILES:** c1ccc2c(c1)ccc1cc3sc4ccccc4c3cc12  
**Mol. weight [g/mol]:** 284.37

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.45		Crippen Method
logp	6.361		Crippen Method
mcvol	211.710	ml/mol	McGowan Method
rinpola	491.02		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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=R21340&Units=SI>

## Legend

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

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