

# 7H-Cyclopenta[1,2-b:3,4-b']dithiophene

**Inchi:** InChI=1S/C9H6S2/c1-3-11-9-6(1)5-8-7(9)2-4-10-8/h1-4H,5H2  
**InchiKey:** XTKJDHXAWHORLK-UHFFFAOYSA-N  
**Formula:** C9H6S2  
**SMILES:** c1cc2c(s1)Cc1ccsc1-2  
**Mol. weight [g/mol]:** 178.27  
**CAS:** 17965-47-8

## Physical Properties

Property code	Value	Unit	Source
ie	7.51	eV	NIST Webbook
ie	7.59	eV	NIST Webbook
log10ws	-3.94		Crippen Method
logp	3.381		Crippen Method
mcvol	120.590	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C17965478&Units=SI>  
**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>

## Legend

**ie:** Ionization energy  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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