

# Benzo[b]naphtho[2,1-d]thiophene, 7-methyl

**Other names:** Benzo[b]naphtho[2,1]thiophene, 7-methyl  
**Inchi:** InChI=1S/C17H12S/c1-11-5-4-8-15-16(11)14-10-9-12-6-2-3-7-13(12)17(14)18-15/h2-10H  
**InchiKey:** QUYZXKGBUUCR-UHFFFAOYSA-N  
**Formula:** C17H12S  
**SMILES:** Cc1cccc2sc3c4ccccc4ccc3c12  
**Mol. weight [g/mol]:** 248.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	5.516		Crippen Method
mcvol	188.900	ml/mol	McGowan Method
rinpol	411.03		NIST Webbook
rinpol	412.08		NIST Webbook
rinpol	412.08		NIST Webbook
rinpol	411.03		NIST Webbook

## Sources

**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=R21251&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

## 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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