

# Benzo[b]naphtho[1,2]thiophene, 3-methyl

**Other names:** Benzo[b]naphtho[1,2-d]thiophene, 3-methyl  
**Inchi:** InChI=1S/C17H12S/c1-11-6-8-13-12(10-11)7-9-16-17(13)14-4-2-3-5-15(14)18-16/h2-10H  
**InchiKey:** UQVGUKYYOUAAMN-UHFFFAOYSA-N  
**Formula:** C17H12S  
**SMILES:** Cc1ccc2c(ccc3sc4cccc4c32)c1  
**Mol. weight [g/mol]:** 248.34  
**CAS:** 84258-63-9

## 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	409.54		NIST Webbook
rinpol	411.48		NIST Webbook
rinpol	409.99		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=C84258639&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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