

# 2-Methyl-4-nonylbenzo[b]thiophene

**Other names:** Benzo[b]thiophene, 2-methyl-4-nonyl  
**Inchi:** InChI=1S/C18H26S/c1-3-4-5-6-7-8-9-11-16-12-10-13-18-17(16)14-15(2)19-18/h10,12-14  
**InchiKey:** NYXKLXMTXBGZRK-UHFFFAOYSA-N  
**Formula:** C18H26S  
**SMILES:** CCCCCCCCCc1cccc2sc(C)cc12  
**Mol. weight [g/mol]:** 274.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.24		Crippen Method
logp	6.503		Crippen Method
mcvol	241.910	ml/mol	McGowan Method
rinpol	2179.00		NIST Webbook
rinpol	2178.60		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2170.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R41623&Units=SI>

## 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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