

# 2-Heptyl-4,5-dimethylthiazole

**Inchi:** InChI=1S/C12H21NS/c1-4-5-6-7-8-9-12-13-10(2)11(3)14-12/h4-9H2,1-3H3  
**InchiKey:** PSZGSWWQPRJONL-UHFFFAOYSA-N  
**Formula:** C12H21NS  
**SMILES:** CCCCCCc1nc(C)c(C)s1  
**Mol. weight [g/mol]:** 211.37

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	4.273		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
rinpol	1588.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1588.00		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=R329996&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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