

# 2-Octyl-4,5-dimethylthiazole

**Inchi:** InChI=1S/C13H23NS/c1-4-5-6-7-8-9-10-13-14-11(2)12(3)15-13/h4-10H2,1-3H3  
**InchiKey:** HGRFDZGIRVFJRV-UHFFFAOYSA-N  
**Formula:** C13H23NS  
**SMILES:** CCCCCCCCc1nc(C)c(C)s1  
**Mol. weight [g/mol]:** 225.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.26		Crippen Method
logp	4.663		Crippen Method
mcvol	200.900	ml/mol	McGowan Method
rinpol	1691.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1692.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R330015&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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