

# 5-ethyl-2-hexyl-thiazole

**Inchi:** InChI=1S/C11H19NS/c1-3-5-6-7-8-11-12-9-10(4-2)13-11/h9H,3-8H2,1-2H3  
**InchiKey:** DAASSIPPQKYXIW-UHFFFAOYSA-N  
**Formula:** C11H19NS  
**SMILES:** CCCCCC1ncc(CC)s1  
**Mol. weight [g/mol]:** 197.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	3.828		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
rinpole	1457.00		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=R498225&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpole:** Non-polar retention indices

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