

# 2(3H)-Benzoxazolethione,3-methyl-

**Other names:** Benzoxazole-2(3H)-thione, 3-methyl-  
**Inchi:** InChI=1S/C8H7NOS/c1-9-6-4-2-3-5-7(6)10-8(9)11/h2-5H,1H3  
**InchiKey:** VMOIPIVQHVUFUFO-UHFFFAOYSA-N  
**Formula:** C8H7NOS  
**SMILES:** Cn1c(=S)oc2ccccc21  
**Mol. weight [g/mol]:** 165.21  
**CAS:** 13673-63-7

## Physical Properties

Property code	Value	Unit	Source
ie	7.94	eV	NIST Webbook
log10ws	-9.15		Crippen Method
logp	2.501		Crippen Method
mcvol	116.860	ml/mol	McGowan Method

## 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=C13673637&Units=SI>

## Legend

**ie:** Ionization energy  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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