# Benzothiazole, 2,6-dimethyl-

**Other names:** 2,6-Dimethylbenzothiazole
**Inchi:** InChI=1S/C9H9NS/c1-6-3-4-8-9(5-6)11-7(2)10-8/h3-5H,1-2H3
**InchiKey:** JEKCSLMWKCKDCC-UHFFFAOYSA-N
**Formula:** C9H9NS
**SMILES:** Cc1ccc2nc(C)sc2c1
**Mol. weight [g/mol]:** 163.24
**CAS:** 2941-71-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -3.75 | | Crippen Method |
| logp | 2.913 | | Crippen Method |
| mcvol | 125.080 | ml/mol | McGowan Method |

## Sources

**Crippen Method:** 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=C2941711&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## Legend

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