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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2941711&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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