

# Benzo[b]thiophene, 2,7-dimethyl-

<b>Other names:</b>	2,7-Dimethylbenzo[b]thiophene 2,7-Dimethyl-1-benzothiophene 2,7-Dimethyl-benzothiophene Benzothiophene, 2,7-dimethyl
<b>Inchi:</b>	InChI=1S/C10H10S/c1-7-4-3-5-9-6-8(2)11-10(7)9/h3-6H,1-2H3
<b>InchiKey:</b>	DNEXCQLUONZSTB-UHFFFAOYSA-N
<b>Formula:</b>	C10H10S
<b>SMILES:</b>	<chem>Cc1cc2cccc(C)c2s1</chem>
<b>Mol. weight [g/mol]:</b>	162.25
<b>CAS:</b>	16587-40-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	3.518		Crippen Method
mcvol	129.190	ml/mol	McGowan Method
rinsol	241.50		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C16587409&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16587409&amp;Units=SI</a>

## Legend

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

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