

# Benzo[b]thiophene, 2-ethyl-5,7-dimethyl-

<b>Other names:</b>	Benzothiophene, 2-ethyl-5,7-dimethyl
<b>Inchi:</b>	InChI=1S/C12H14S/c1-4-11-7-10-6-8(2)5-9(3)12(10)13-11/h5-7H,4H2,1-3H3
<b>InchiKey:</b>	SEUHVQFYOBCERO-UHFFFAOYSA-N
<b>Formula:</b>	C12H14S
<b>SMILES:</b>	CCc1cc2cc(C)cc(C)c2s1
<b>Mol. weight [g/mol]:</b>	190.31
<b>CAS:</b>	18428-05-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	4.081		Crippen Method
mcvol	157.370	ml/mol	McGowan Method
rinpola	1719.00		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=C18428052&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18428052&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>rinpola:</b>	Non-polar retention indices

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