

# 2,3,6-Trimethyl-benzo-[b]-furan

<b>Inchi:</b>	InChI=1S/C11H12O/c1-7-4-5-10-8(2)9(3)12-11(10)6-7/h4-6H,1-3H3
<b>InchiKey:</b>	JHWKKCNDPCOCDL-UHFFFAOYSA-N
<b>Formula:</b>	C11H12O
<b>SMILES:</b>	Cc1ccc2c(C)c(C)oc2c1
<b>Mol. weight [g/mol]:</b>	160.21

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.44		Crippen Method
logp	3.358		Crippen Method
mcvol	132.800	ml/mol	McGowan Method
ripol	1822.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R326086&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R326086&amp;Units=SI</a>
<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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>ripol:</b>	Polar retention indices

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