

# 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>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=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>                                 |

## 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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