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

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R326086&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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