5,6-Dihydro-3,6-dimethyl-benzo-[b]-furan-7(4H)-or

Inchi: InChI=1S/C10H12O2/c1-6-3-4-8-7(2)5-12-10(8)9(6)11/h5-6H,3-4H2,1-2H3
InchiKey: NOBIKWOTCGZIEF-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: Cc1coc2c1CCC(C)C2=O
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.22		Crippen Method
logp	2.353		Crippen Method
mcvol	128.880	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R326239&Units=SI

Legend

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