

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

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/ci9903071
Crippen Method:	https://www.cheméo.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

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