Benzofuran, 2,3-dimethyl-7-methoxy

Inchi: InChI=1S/C11H12O2/c1-7-8(2)13-11-9(7)5-4-6-10(11)12-3/h4-6H,1-3H3
InchiKey: AVNATQPOCOKYSF-UHFFFAOYSA-N
Formula: C11H12O2
SMILES: COc1cccc2c(C)c(C)oc12
Mol. weight [g/mol]: 176.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.08		Crippen Method
logp	3.058		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
rinpol	1481.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R521543&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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