

2-Methyl-5-methoxybenzofuran

Other names: 5-Methoxy-2-methylbenzofuran
Inchi: InChI=1S/C10H10O2/c1-7-5-8-6-9(11-2)3-4-10(8)12-7/h3-6H,1-2H3
InchiKey: IKUBQGOYKPKCKQ-UHFFFAOYSA-N
Formula: C10H10O2
SMILES: COc1ccc2oc(C)cc2c1
Mol. weight [g/mol]: 162.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.61		Crippen Method
logp	2.750		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
rinpol	1336.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1336.00		NIST Webbook
ripol	2060.00		NIST Webbook
ripol	2060.00		NIST Webbook
ripol	2060.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R240096&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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

ripol: Polar retention indices

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