

Benzofuran, 4,7-dimethyl-

Other names:	4,7-Dimethylbenzofuran
Inchi:	InChI=1S/C10H10O/c1-7-3-4-8(2)10-9(7)5-6-11-10/h3-6H,1-2H3
InchiKey:	PFXVPEGRXODMIQ-UHFFFAOYSA-N
Formula:	C10H10O
SMILES:	Cc1ccc(C)c2occc12
Mol. weight [g/mol]:	146.19
CAS:	28715-26-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.96		Crippen Method
logp	3.050		Crippen Method
mcvol	118.710	ml/mol	McGowan Method
rinpol	1220.00		NIST Webbook
rinpol	1220.40		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1220.40		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1218.00		NIST Webbook

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=C28715266&Units=SI

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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