

Benzofuran, 3-methyl-

Other names:	3-Methyl-benzofuran
Inchi:	InChI=1S/C9H8O/c1-7-6-10-9-5-3-2-4-8(7)9/h2-6H,1H3
InchiKey:	ZRXHLJNBNWVNIM-UHFFFAOYSA-N
Formula:	C9H8O
SMILES:	Cc1coc2ccccc12
Mol. weight [g/mol]:	132.16
CAS:	21535-97-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.49		Crippen Method
logp	2.741		Crippen Method
mcvol	104.620	ml/mol	McGowan Method
rinpol	181.10		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=C21535977&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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<https://www.chemeo.com/cid/10-137-8/Benzofuran-3-methyl.pdf>

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