

Benzofuran, 7-methoxy-

Other names:	7-Methoxybenzofuran
Inchi:	InChI=1S/C9H8O2/c1-10-8-4-2-3-7-5-6-11-9(7)8/h2-6H,1H3
InchiKey:	QPLLPLLBBSWRM-UHFFFAOYSA-N
Formula:	C9H8O2
SMILES:	COc1cccc2ccoc12
Mol. weight [g/mol]:	148.16
CAS:	7168-85-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.13		Crippen Method
logp	2.441		Crippen Method
mcvol	110.490	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C7168856&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/33-425-3/Benzofuran-7-methoxy.pdf>

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