Benzofuran, 7-methyl-

Other names:	7-Methylbenzofuran
	7-Methylbenzo[b]furan
Inchi:	InChI=1S/C9H8O/c1-7-3-2-4-8-5-6-10-9(7)8/h2-6H,1H3
InchiKey:	PHQXPPBIJBCIMI-UHFFFAOYSA-N
Formula:	C9H8O
SMILES:	Cc1cccc2ccoc12
Mol. weight [g/mol]:	132.16
CAS:	17059-52-8

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	181.80		NIST Webbook
rinpol	182.10		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17059528&Units=SI
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

Legend

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

Latest version available from:

https://www.chemeo.com/cid/10-316-9/Benzofuran-7-methyl.pdf

Generated by Cheméo on 2024-10-12 05:34:19.383009756 +0000 UTC m=+3292122.019979005.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.