

4-methyl-2-vinylfuran

Inchi:	InChI=1S/C7H8O/c1-3-7-4-6(2)5-8-7/h3-5H,1H2,2H3
InchiKey:	XKLXIAXQKXXTMR-UHFFFAOYSA-N
Formula:	C7H8O
SMILES:	C=Cc1cc(C)co1
Mol. weight [g/mol]:	108.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.50		Crippen Method
logp	2.231		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
ripol	1218.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R491571&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol:	Polar retention indices

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<https://www.chemeo.com/cid/77-883-7/4-methyl-2-vinylfuran.pdf>

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