

Furan, 3-(1-methyl-1,4-pentadien-1-yl)

Other names:	Furan, 3-(1-methyl-1,4-pentadienyl)
Inchi:	InChI=1S/C10H12O/c1-3-4-5-9(2)10-6-7-11-8-10/h3,5-8H,1,4H2,2H3/b9-5+
InchiKey:	NEWCDYUSODCGMO-WEVVVXLNSA-N
Formula:	C10H12O
SMILES:	C=CCC=C(C)c1ccoc1
Mol. weight [g/mol]:	148.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.56		Crippen Method
logp	3.259		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
rinpol	1083.00		NIST Webbook
rinpol	1083.00		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=R324897&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

Latest version available from:

<https://www.chemeo.com/cid/60-696-3/Furan-3-1-methyl-1-4-pentadien-1-yl.pdf>

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