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