

2-(5-methyl-2-furanyl)furan

Inchi: InChI=1S/C9H8O2/c1-7-4-5-9(11-7)8-3-2-6-10-8/h2-6H,1H3
InchiKey: ZGQUDOQDKZDRQB-UHFFFAOYSA-N
Formula: C9H8O2
SMILES: Cc1ccc(-c2ccco2)o1
Mol. weight [g/mol]: 148.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.02		Crippen Method
logp	2.848		Crippen Method
mcvol	110.490	ml/mol	McGowan Method
ripol	1656.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1656.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R491526&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/92-355-6/2-5-methyl-2-furanyl-furan.pdf>

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