

2-(4-methyl-2-furfuryl)furan

Inchi: InChI=1S/C10H10O2/c1-8-5-10(12-7-8)6-9-3-2-4-11-9/h2-5,7H,6H2,1H3
InchiKey: IRVRGTIXQZWORH-UHFFFAOYSA-N
Formula: C10H10O2
SMILES: Cc1coc(Cc2cccO2)c1
Mol. weight [g/mol]: 162.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.52		Crippen Method
logp	2.772		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
ripol	1683.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1684.00		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=R491511&Units=SI>

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/94-413-9/2-4-methyl-2-furfuryl-furan.pdf>

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