2-(3-methyl-2-furfuryl)furan

Inchi: InChI=1S/C10H10O2/c1-8-4-6-12-10(8)7-9-3-2-5-11-9/h2-6H,7H2,1H3
InchiKey: KLVKIZHAZBULQX-UHFFFAOYSA-N
Formula: C10H10O2
SMILES: Cc1ccoc1Cc1ccco1
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
ripol	1684.00		NIST Webbook
ripol	1683.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R491506&Units=SI
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

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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