

2-methyl-3-[(2-furyl-methyl)thio]furan

Other names: 2-methyl-3-[(2-furanylmethyl)thio]furan
Inchi: InChI=1S/C10H10O2S/c1-8-10(4-6-11-8)13-7-9-3-2-5-12-9/h2-6H,7H2,1H3
InchiKey: BNWGBSRYEZEHNX-UHFFFAOYSA-N
Formula: C10H10O2S
SMILES: Cc1occc1SCc1ccco1
Mol. weight [g/mol]: 194.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.27		Crippen Method
logp	3.473		Crippen Method
mcvol	140.930	ml/mol	McGowan Method
rinpol	1503.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1503.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R223031&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
rinpol: Non-polar retention indices

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