2-Methyl-3-[(2-methylbutyl)-thio]-furan

Inchi: InChI=1S/C10H16OS/c1-4-8(2)7-12-10-5-6-11-9(10)3/h5-6,8H,4,7H2,1-3H3
InchiKey: BPCVNFWIMVTFOL-UHFFFAOYSA-N
Formula: C10H16OS
SMILES: CCC(C)CSc1ccoc1C
Mol. weight [g/mol]: 184.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.86		Crippen Method
logp	3.726		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
rinpol	1250.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1250.00		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=U360328&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