2-methyl-5-[(methylthio)methyl]furan

Inchi: InChI=1S/C7H10OS/c1-6-3-4-7(8-6)5-9-2/h3-4H,5H2,1-2H3
InchiKey: WFHOSUSADRVYLU-UHFFFAOYSA-N
Formula: C7H10OS
SMILES: CSCc1ccc(C)o1
Mol. weight [g/mol]: 142.22
CAS: 13679-60-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.86		Crippen Method
logp	2.451		Crippen Method
mcvol	112.250	ml/mol	McGowan Method
rinpol	1080.00		NIST Webbook
rinpol	1080.00		NIST Webbook
ripol	1531.00		NIST Webbook
ripol	1531.00		NIST Webbook

Sources

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=C13679602&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices