

Methyl 2-ethyl furyl sulfide

Inchi: InChI=1S/C7H10OS/c1-3-6-4-5-8-7(6)9-2/h4-5H,3H2,1-2H3
InchiKey: REXKADWSAWFKLV-UHFFFAOYSA-N
Formula: C7H10OS
SMILES: CCc1ccoc1SC
Mol. weight [g/mol]: 142.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.75		Crippen Method
logp	2.564		Crippen Method
mcvol	112.250	ml/mol	McGowan Method
ripol	1543.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1543.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R306666&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/81-138-9/Methyl-2-ethyl-furyl-sulfide.pdf>

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