S-(5-methyl-2-furfuryl)thioacetate

Inchi: InChI=1S/C8H10O2S/c1-6-3-4-8(10-6)5-11-7(2)9/h3-4H,5H2,1-2H3
InchiKey: XRURGDZLDVEQRB-UHFFFAOYSA-N
Formula: C8H10O2S
SMILES: CC(=O)SCc1ccc(C)o1
Mol. weight [g/mol]: 170.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.06		Crippen Method
logp	2.368		Crippen Method
mcvol	127.910	ml/mol	McGowan Method
ripol	1840.00		NIST Webbook
ripol	1840.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R336464&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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