

2-[(methyltrithio)methyl]furan

Other names: 2-furfuryl methyl trisulfide
Inchi: InChI=1S/C6H8OS3/c1-8-10-9-5-6-3-2-4-7-6/h2-4H,5H2,1H3
InchiKey: ORKOECRFEGYATC-UHFFFAOYSA-N
Formula: C6H8OS3
SMILES: CSSSCc1ccco1
Mol. weight [g/mol]: 192.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.14		Crippen Method
logp	3.439		Crippen Method
mcvol	130.860	ml/mol	McGowan Method
rinpol	1475.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1490.00		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=R227711&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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