

# 1-[(2-methyl-3-furyl)dithio]-2-propanone

**Other names:** 2-Propanone, 1-(2-methyl-3-furyldithio)  
**Inchi:** InChI=1S/C8H10O2S2/c1-6(9)5-11-12-8-3-4-10-7(8)2/h3-4H,5H2,1-2H3  
**InchiKey:** FAADBWMWDANEGB-UHFFFAOYSA-N  
**Formula:** C8H10O2S2  
**SMILES:** CC(=O)CSSc1ccoc1C  
**Mol. weight [g/mol]:** 202.29

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.42		Crippen Method
logp	2.917		Crippen Method
mcvol	144.260	ml/mol	McGowan Method
rinpol	1476.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1462.00		NIST Webbook
ripol	2235.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2235.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=U357166&Units=SI>

# Legend

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

Latest version available from:

<https://www.cheméo.com/cid/121-870-1/1-2-methyl-3-furyl-dithio-2-propanone.pdf>

Generated by Cheméo on 2024-04-30 21:42:43.573676945 +0000 UTC m=+16802612.494254258.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.