# 2-furfuryl 2-oxo-3-butyl disulfide

**Other names:** 3-[(2-Furylmethyl)dithio]-2-butanone
**Inchi:** InChI=1S/C9H12O2S2/c1-7(10)8(2)13-12-6-9-4-3-5-11-9/h3-5,8H,6H2,1-2H3
**InchiKey:** LOGIPTDAOGQBBJ-UHFFFAOYSA-N
**Formula:** C9H12O2S2
**SMILES:** CC(=O)C(C)SSCc1ccco1
**Mol. weight [g/mol]:** 216.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -7.91 | | Crippen Method |
| logp | 3.138 | | Crippen Method |
| mcvol | 158.350 | ml/mol | McGowan Method |
| rinpol | 1589.00 | | NIST Webbook |
| rinpol | 1604.00 | | NIST Webbook |
| rinpol | 1577.00 | | NIST Webbook |
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| rinpol | 1577.00 | | NIST Webbook |
| rinpol | 1589.00 | | NIST Webbook |
| ripol | 2352.00 | | NIST Webbook |
| ripol | 2352.00 | | NIST Webbook |
| ripol | 2352.00 | | NIST Webbook |

## Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U365960&Units=SI

## 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 |