

# 2-Furanthiol

**Other names:** furan-2-thiol  
**Inchi:** InChI=1S/C4H4OS/c6-4-2-1-3-5-4/h1-3,6H  
**InchiKey:** CMDKYFGIJALPLS-UHFFFAOYSA-N  
**Formula:** C4H4OS  
**SMILES:** Sc1ccco1  
**Mol. weight [g/mol]:** 100.14  
**CAS:** 13129-35-6

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.72   |        | Crippen Method |
| logp          | 1.568   |        | Crippen Method |
| mcvol         | 69.980  | ml/mol | McGowan Method |
| rinpol        | 912.00  |        | NIST Webbook   |
| rinpol        | 912.00  |        | NIST Webbook   |
| rinpol        | 914.00  |        | NIST Webbook   |
| rinpol        | 914.00  |        | NIST Webbook   |
| ripol         | 1443.00 |        | NIST Webbook   |
| ripol         | 1443.00 |        | NIST Webbook   |

## Sources

**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=C13129356&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  
**ripol:** Polar retention indices

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