# 2-Furancarbothioic acid, S-methyl ester

| | |
|---|---|
| **Other names:** | 2-Furoic acid, thio-, S-methyl ester |
| | Methyl 2-thiofuroate |
| | Methylthiol furoate |
| | S-Methyl thiofuroate |
| | S-Methyl 2-furancarbothioate |
| | Methyl thiofuroate |
| | methyl thio-2-furoate |
| **Inchi:** | InChI=1S/C6H6O2S/c1-9-6(7)5-3-2-4-8-5/h2-4H,1H3 |
| **InchiKey:** | ISKUAGFDTRLBHG-UHFFFAOYSA-N |
| **Formula:** | C6H6O2S |
| **SMILES:** | CSC(=O)c1ccco1 |
| **Mol. weight [g/mol]:** | 142.18 |
| **CAS:** | 13679-61-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -6.24 | | Crippen Method |
| logp | 1.783 | | Crippen Method |
| mcvol | 99.730 | ml/mol | McGowan Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C13679613&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