

3H-1,2-Dithiole-3-thione, 4-methyl-

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C4H4S3/c1-3-2-6-7-4(3)5/h2H,1H3 |
| InchiKey: | YHKZVQYBNUVXKY-UHFFFAOYSA-N |
| Formula: | C4H4S3 |
| SMILES: | Cc1cssc1=S |
| Mol. weight [g/mol]: | 148.27 |
| CAS: | 3354-41-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| ie | 8.23 | eV | NIST Webbook |
| log10ws | -2.31 | | Crippen Method |
| logp | 2.848 | | Crippen Method |
| mcvol | 96.810 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3354414&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

| | |
|-----------------|-------------------------------------|
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

Latest version available from:

<https://www.chemeo.com/cid/65-796-7/3H-1-2-Dithiole-3-thione-4-methyl.pdf>

Generated by Cheméo on 2024-04-28 22:13:47.933206763 +0000 UTC m=+16631676.853784075.

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