

4(1H)-Pyrimidinone, 2,3-dihydro-2-thioxo-6-(trifluoromethyl)-

| | |
|----------------------|---|
| Other names: | Uracil, 2-thio-6-(trifluoromethyl)- 2-Mercapto-6-(trifluoromethyl)pyrimidin-4-ol |
| Inchi: | InChI=1S/C5H3F3N2OS/c6-5(7,8)2-1-3(11)10-4(12)9-2/h1H,(H2,9,10,11,12) |
| InchiKey: | YZAOETRYQWFEOY-UHFFFAOYSA-N |
| Formula: | C5H3F3N2OS |
| SMILES: | Oc1cc(C(F)(F)F)nc(S)n1 |
| Mol. weight [g/mol]: | 196.15 |
| CAS: | 368-54-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.17 | | Crippen Method |
| logp | 1.490 | | Crippen Method |
| mcvol | 105.040 | ml/mol | McGowan Method |

Sources

| | |
|-----------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C368547&Units=SI |

Legend

| | |
|----------|-------------------------------------|
| 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/116-075-0/4-1H-Pyrimidinone-2-3-dihydro-2-thioxo-6-trifluoromethyl.pdf>

Generated by Cheméo on 2024-05-03 12:23:01.621131852 +0000 UTC m=+17028230.541709164.

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