

# 2,4(1H,3H)-Pyrimidinedithione

<b>Other names:</b>	Uracil, 2,4-dithio- Dithiouracil 2,4-Dimercaptopyrimidine 2,4-Dithiouracil 2,4-Dithioxopyrimidine 2,4-Pyrimidinedithiol Pyrimidine-2,4-dithiol 2,4-Dithiopyrimidine Dithiopyrimidine USAF CB-14 NSC 42031
<b>Inchi:</b>	InChI=1S/C4H4N2S2/c7-3-1-2-5-4(8)6-3/h1-2H,(H2,5,6,7,8)
<b>InchiKey:</b>	ZEQIWKHCJWRNTH-UHFFFAOYSA-N
<b>Formula:</b>	C4H4N2S2
<b>SMILES:</b>	Sc1ccnc(S)n1
<b>Mol. weight [g/mol]:</b>	144.22
<b>CAS:</b>	2001-93-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	1.054		Crippen Method
mcvol	96.120	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2001936&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2001936&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

# 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.cheméo.com/cid/98-321-7/2-4-1H-3H-Pyrimidinedithione.pdf>

Generated by Cheméo on 2024-04-23 18:09:59.821583247 +0000 UTC m=+16185048.742160562.

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