

Methylthiouracil

Other names:

- 2,3-Dihydro-6-methyl-2-thioxo-4(1H)-pyrimidinone
- 2-Mercapto-4-hydroxy-6-methylpyrimidine
- 2-Mercapto-6-methyl-4-pyrimidinol
- 2-Mercapto-6-methyl-4-pyrimidone
- 2-Mercapto-6-methylpyrimid-4-one
- 2-Thio-4-oxo-6-methyl-1,3-pyrimidine
- 2-Thio-6-methyl-1,3-pyrimidin-4-one
- 2-Thio-6-methyluracil
- 2-Thiouracil, 6-methyl-
- 4(1H)-Pyrimidinone, 2,3-dihydro-6-methyl-2-thioxo-
- 4-Hydroxy-2-mercapto-6-methylpyrimidine
- 4-Hydroxy-6-methyl-2-thiopyrimidine
- 4-Methyl-2-thiouracil
- 6-Methyl-2-mercaptouracil
- 6-Methyl-2-thio-2,4(1H,3H)-pyrimidinedione
- 6-Methyl-2-thiouracil
- 6-Methyl-2-thiouracyl
- 6-Methyl-4-oxo-2-thioxo-1,2,3,4-tetrahydropyrimidine
- 6-Methylthiouracil
- 6-Metil-tiouracile
- 6-Thio-4-methyluracil
- Alkiron
- Basecil
- Basethyrin
- MTU
- Metacil
- Methacil
- Methiacil
- Methicil
- Methiocil
- Metiur
- Muracil
- Muracin
- NSC 193526
- NSC 9378
- Orcanon
- Prostrumyl
- RCRA Waste number U164
- Strumacil
- Thimecil

Thiomecil
 Thiomidil
 Thioryl
 Thiothymin
 Thiothyron
 Thiuryl
 Thyreonorm
 Thyreostat
 Thyreostat I
 Thyril
 Tiomeracil
 Tiorale M
 Tiotiron
 USAF EK-6454
 Uracil, 6-methyl-2-thio-
 antiBason

Inchi: InChI=1S/C5H6N2OS/c1-3-2-4(8)7-5(9)6-3/h2H,1H3,(H2,6,7,8,9)
InchiKey: HWGBHCRJGXAGEU-UHFFFAOYSA-N
Formula: C5H6N2OS
SMILES: Cc1cc(O)nc(S)n1
Mol. weight [g/mol]: 142.18
CAS: 56-04-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	0.779		Crippen Method
mvol	99.730	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
psub	1.06e-04	kPa	421.16	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

psub	1.24e-04	kPa	423.15	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	1.36e-04	kPa	425.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	1.82e-04	kPa	427.16	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.15e-04	kPa	429.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.47e-04	kPa	431.19	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.47e-04	kPa	431.16	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.91e-04	kPa	433.20	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	3.42e-04	kPa	435.22	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

psub	4.05e-04	kPa	437.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	4.69e-04	kPa	439.22	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	5.62e-04	kPa	441.23	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	4.18e-04	kPa	437.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	5.28e-04	kPa	439.20	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	6.92e-04	kPa	443.16	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	8.13e-04	kPa	445.21	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	9.50e-04	kPa	447.24	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	6.89e-04	kPa	443.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

psub	9.52e-04	kPa	447.24	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	1.24e-04	kPa	423.15	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	1.45e-04	kPa	425.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	1.62e-04	kPa	427.16	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.14e-04	kPa	429.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.53e-04	kPa	431.19	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.89e-04	kPa	433.20	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	3.42e-04	kPa	435.22	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

psub	3.98e-04	kPa	437.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	4.78e-04	kPa	439.22	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	5.64e-04	kPa	441.23	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	4.97e-04	kPa	439.20	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	5.89e-04	kPa	441.23	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	8.06e-04	kPa	445.21	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	9.41e-04	kPa	447.24	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	7.98e-04	kPa	445.20	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	9.49e-04	kPa	447.24	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

psub	9.78e-05	kPa	421.16	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	1.20e-04	kPa	423.15	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	1.41e-04	kPa	425.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	1.71e-04	kPa	427.16	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.00e-04	kPa	429.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.43e-04	kPa	431.19	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.30e-04	kPa	431.16	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.71e-04	kPa	433.20	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

psub	3.33e-04	kPa	435.22	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	3.85e-04	kPa	437.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	4.52e-04	kPa	439.22	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	5.43e-04	kPa	441.23	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	4.05e-04	kPa	437.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	4.80e-04	kPa	439.20	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	5.73e-04	kPa	441.23	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	6.45e-04	kPa	443.16	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	7.57e-04	kPa	445.21	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

psub	9.09e-04	kPa	447.24	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	6.57e-04	kPa	443.17	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	7.79e-04	kPa	445.20	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	9.23e-04	kPa	447.24	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C56042&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil in aqueous co-solvent mixtures of methanol, N-methyl-2-pyrrolidone, N,N-dimethyl formamide and dimethyl sulfoxide:

<https://www.doi.org/10.1016/j.jct.2012.08.004>

<https://www.doi.org/10.1016/j.jct.2018.02.002>

Legend

- log10ws:** Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
psub: Sublimation pressure

Latest version available from:

<https://www.cheméo.com/cid/18-005-6/Methylthiouracil.pdf>

Generated by Cheméo on 2024-04-20 13:36:37.634895715 +0000 UTC m=+15909446.555473027.

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