

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-mercaptopuracil
	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
Thyрил
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
mcvol	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

Crippen Method:

Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil. Equilibrium solubility, dissolution thermodynamics and preferential solvation of 6-methyl-2-thiouracil in aqueous co-solvent mixtures of methanol, N-methyl-2-pyrrolidone, N,N-dimethyl formamide and dimethylsulfoxide.

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

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

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

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

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

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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.chemeo.com/cid/18-005-6/Methylthiouracil.pdf>

Generated by Cheméo on 2024-05-02 22:15:29.032532036 +0000 UTC m=+16977377.953109357.

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