

5-METHYL-2-THIOXO-2,3-DIHYDRO-4(1H)-PYRIMIDINE

Other names:	2-Thiothymine 5-Methyl-2-thiouracil Thiothymine Thymine, 2-thio- Uracil, 5-methyl-2-thio-
Inchi:	InChI=1S/C5H6N2OS/c1-3-2-6-5(9)7-4(3)8/h2H,1H3,(H2,6,7,8,9)
InchiKey:	ZLAQATDNGLKIEV-UHFFFAOYSA-N
Formula:	C5H6N2OS
SMILES:	Cc1c[nH]c(=S)[nH]c1=O
Mol. weight [g/mol]:	142.18

Physical Properties

Property code	Value	Unit	Source
hf	-76.35	kJ/mol	Cheméo Relay (1.0)
hvap	127.01	kJ/mol	Cheméo Relay (1.0)
ie	8.11	eV	Cheméo Relay (1.0)
log10ws	-1.38		Cheméo Relay (1.0)
logp	-0.223		Crippen Method
mcvol	99.730	ml/mol	McGowan Method
tf	505.98	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
psub	1.77e-04	kPa	413.15	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.17e-04	kPa	415.25	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

psub	3.13e-04	kPa	419.23	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	3.74e-04	kPa	421.24	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	4.42e-04	kPa	423.16	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	5.10e-04	kPa	425.20	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	6.26e-04	kPa	427.22	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	7.52e-04	kPa	429.15	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	8.52e-04	kPa	431.22	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	1.05e-03	kPa	433.24	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	1.70e-04	kPa	413.15	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

psub	2.11e-04	kPa	415.25	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.54e-04	kPa	417.15	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	3.13e-04	kPa	419.23	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	4.36e-04	kPa	423.16	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	5.30e-04	kPa	425.20	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	6.12e-04	kPa	427.22	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	7.32e-04	kPa	429.15	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	8.69e-04	kPa	431.22	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

psub	1.03e-03	kPa	433.24	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.10e-04	kPa	415.25	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.51e-04	kPa	417.24	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	2.50e-04	kPa	417.15	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	3.02e-04	kPa	419.23	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	3.61e-04	kPa	421.24	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	4.21e-04	kPa	423.16	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	5.05e-04	kPa	425.20	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	6.01e-04	kPa	427.22	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

psub	7.07e-04	kPa	429.15	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	8.41e-04	kPa	431.22	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil
psub	1.02e-03	kPa	433.24	Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C636260&Units=SI>

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

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Experimental study on the thermochemistry of 2-thiouracil, 5-methyl-2-thiouracil and 6-methyl-2-thiouracil: <https://www.doi.org/10.1016/j.jct.2012.08.004>

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
psub:	Sublimation pressure
tf:	Normal melting (fusion) point

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