5,6-Dihydro-6-methyluracil

Other names:	2,4(1H,3H)-Pyrimidinedione, dihydro-6-methyl- 4-Methyldihydrouracil 5,6-dihydro-5-methyluracil 5,6-dihydrothymine 5-methyl-5,6-dihydrouracil 5-methyldihydropyrimidine-2,4(1H,3H)-dione 5-methylhydrouracil 6-Methyl-5,6-dihydrouracil 6-Methyldihydro-2,4(1H,3H)-pyrimidinedione 6-Methyldihydrouracil Dihydro-6-methyluracil Hydrouracil, 6-methyl- Metacil, dihydro- NSC 44127
Inchi:	InChI=1S/C5H8N2O2/c1-3-2-4(8)7-5(9)6-3/h3H,2H2,1H3,(H2,6,7,8,9)
InchiKey:	XQLIRTZXJDEQAO-UHFFFAOYSA-N
Formula:	C5H8N2O2
SMILES:	CC1CC(=O)NC(=O)N1
Mol. weight [g/mol]:	128.13
CAS:	2434-49-3

Physical Properties

Property code	Value	Unit	Source
chs	-2592.40	kJ/mol	NIST Webbook
chs	-2592.00	kJ/mol	NIST Webbook
gf	-54.09	kJ/mol	Joback Method
hf	-291.99	kJ/mol	Joback Method
hfus	18.74	kJ/mol	Joback Method
hvap	49.16	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	-0.396		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	5304.68	kPa	Joback Method
tb	566.09	K	Joback Method
tc	826.71	K	Joback Method
tf	499.99	K	Joback Method
vc	0.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.01	J/mol×K	826.71	Joback Method
cpg	284.87	J/mol×K	783.28	Joback Method
cpg	273.71	J/mol×K	739.84	Joback Method
cpg	261.65	J/mol×K	696.40	Joback Method
cpg	248.80	J/mol×K	652.96	Joback Method
cpg	235.27	J/mol×K	609.53	Joback Method
cpg	221.19	J/mol×K	566.09	Joback Method
psub	7.56e-04	kPa	397.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	6.32e-04	kPa	395.16	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	7.86e-04	kPa	397.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	9.06e-04	kPa	399.19	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	1.11e-03	kPa	401.16	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	1.31e-04	kPa	379.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	1.63e-04	kPa	381.18	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	1.97e-04	kPa	383.14	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil

psub	2.42e-04	kPa	385.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	2.98e-04	kPa	387.19	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	3.59e-04	kPa	389.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	4.27e-04	kPa	391.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	5.21e-04	kPa	393.19	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	6.33e-04	kPa	395.16	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	5.38e-04	kPa	393.19	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	9.51e-04	kPa	399.19	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	1.10e-03	kPa	401.16	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	1.27e-04	kPa	379.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	1.57e-04	kPa	381.18	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	1.90e-04	kPa	383.14	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil

psub	2.34e-04	kPa	385.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	2.87e-04	kPa	387.19	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	3.46e-04	kPa	389.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	4.20e-04	kPa	391.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	5.08e-04	kPa	393.19	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	6.13e-04	kPa	395.16	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	7.37e-04	kPa	397.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	8.82e-04	kPa	399.19	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	1.07e-03	kPa	401.16	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	4.42e-04	kPa	391.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	3.64e-04	kPa	389.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	3.01e-04	kPa	387.19	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil

psub	2.43e-04	kPa	385.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	1.98e-04	kPa	383.14	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	1.68e-04	kPa	381.18	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil
psub	1.38e-04	kPa	379.15	Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2434493&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpies of formation of 5,6-dihydro-5-methyluracil and 5,6-dihydro-6-methyluracil:	https://www.doi.org/10.1016/j.jct.2013.05.002
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume