

5,6-Dihydro-5-methyluracil

Other names:	5,6-Dihydro-2,4-dihydroxy-5-methylpyrimidine Dihydrothymine 2,4(1H,3H)-Pyrimidinedione, dihydro-5-methyl- Hydrouracil, 5-methyl- 5-Methyl-5,6-dihydrouracil 5,6-Dihydrothymine
Inchi:	InChI=1S/C5H8N2O2/c1-3-2-6-5(9)7-4(3)8/h3H,2H2,1H3,(H2,6,7,8,9)
InchiKey:	NBAKTGXDIBVZOO-UHFFFAOYSA-N
Formula:	C5H8N2O2
SMILES:	CC1CNC(=O)NC1=O
Mol. weight [g/mol]:	128.13
CAS:	696-04-8

Physical Properties

Property code	Value	Unit	Source
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	-0.48		Crippen Method
logp	-0.538		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	5304.68	kPa	Joback Method
rinpol	1523.80		NIST Webbook
rinpol	1523.80		NIST Webbook
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	221.19	J/molxK	566.09	Joback Method

cpg	235.27	J/mol×K	609.53	Joback Method
cpg	248.80	J/mol×K	652.96	Joback Method
cpg	261.65	J/mol×K	696.40	Joback Method
cpg	273.71	J/mol×K	739.84	Joback Method
cpg	284.87	J/mol×K	783.28	Joback Method
cpg	295.01	J/mol×K	826.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C696048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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