

2,4(1H,3H)-Pyrimidinedione, dihydro-

Other names:	Hydrouracil Dihydrouracil 5,6-Dihydro-2,4-dihydroxypyrimidine 5,6-Dihydrouracil Dihydro-2,4(1H,3H)-pyrimidinedione Dihydro-pyrimidine-2,4-dione
Inchi:	InChI=1S/C4H6N2O2/c7-3-1-2-5-4(8)6-3/h1-2H2,(H2,5,6,7,8)
InchiKey:	OIVLITBTBDPEFK-UHFFFAOYSA-N
Formula:	C4H6N2O2
SMILES:	O=C1CCNC(=O)N1
Mol. weight [g/mol]:	114.10
CAS:	504-07-4

Physical Properties

Property code	Value	Unit	Source
gf	-54.80	kJ/mol	Joback Method
hf	-251.01	kJ/mol	Joback Method
hfus	15.08	kJ/mol	Joback Method
hvap	47.25	kJ/mol	Joback Method
ie	10.00	eV	NIST Webbook
ie	10.00 ± 0.10	eV	NIST Webbook
log10ws	-0.30		Crippen Method
logp	-0.784		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	6461.89	kPa	Joback Method
tb	547.88	K	Joback Method
tc	814.53	K	Joback Method
tf	492.96	K	Joback Method
vc	0.281	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.96	J/mol×K	547.88	Joback Method

cpg	187.18	J/mol×K	592.32	Joback Method
cpg	198.97	J/mol×K	636.76	Joback Method
cpg	210.22	J/mol×K	681.20	Joback Method
cpg	220.81	J/mol×K	725.65	Joback Method
cpg	230.64	J/mol×K	770.09	Joback Method
cpg	239.58	J/mol×K	814.53	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C504074&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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