5-CHLOROURACIL

Other names:	Uracil, 5-chloro- 5-Chlorouracil
Inchi:	InChI=1S/C4H3ClN2O2/c5-2-1-6-4(9)7-3(2)8/h1H,(H2,6,7,8,9)
InchiKey:	ZFTBZKVVGZNMJR-UHFFFAOYSA-N
Formula:	C4H3ClN2O2
SMILES:	O=c1[nH]cc(Cl)c(=O)[nH]1
Mol. weight [g/mol]:	146.53

Physical Properties

Property code	Value	Unit	Source
hf	-291.29	kJ/mol	Cheméo Relay (1.0)
hsub	148.30 ± 2.40	kJ/mol	NIST Webbook
hvap	99.39	kJ/mol	Cheméo Relay (1.0)
ie	9.33	eV	Cheméo Relay (1.0)
log10ws	-0.76		Cheméo Relay (1.0)
logp	-1.247		Crippen Method
mcvol	87.400	ml/mol	McGowan Method
tf	484.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	145.50	kJ/mol	407.00	NIST Webbook

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1820811&Units=SI

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

Legend

hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tf:	Normal melting (fusion) point