2,4(1H,3H)-Pyrimidinedione, 1,3,5-trimethyl-

Other names: Uracil, 1,3,5-trimethyl-
1,3-Dimethylthymine
Inchi: InChI=1S/C7H10N2O2/c1-5-4-8(2)7(11)9(3)6(5)10/h4H,1-3H3
InchiKey: BHWQEVXICGSHEW-UHFFFAOYSA-N
Formula: C7H10N2O2
SMILES: Cc1cn(C)c(=O)n(C)c1=O
Mol. weight [g/mol]: 154.17
CAS: 4401-71-2

Physical Properties

Property code	Value	Unit	Source
ie	8.30 ± 0.10	eV	NIST Webbook
log10ws	-3.37		Crippen Method
logp	-0.608		Crippen Method
mcvol	117.430	ml/mol	McGowan Method
tf	426.50 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	16.10	kJ/mol	428.70	NIST Webbook
hsubt	103.50 ± 1.50	kJ/mol	326.00	NIST Webbook
hsubt	109.20 ± 2.10	kJ/mol	338.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4401712&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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