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

Other names:	Uracil, 5-bromo-
	Bromouracil
	5-Bromouracil
	5-Bromo-2,4-dihydroxypyrimidine
	2,4-Pyrimidinedione, 1,2,3,4-tetrahydro-5-bromo
Inchi:	InChI=1S/C4H3BrN2O2/c5-2-1-6-4(9)7-3(2)8/h1H,(H2,6,7,8,9)
InchiKey:	LQLQRFGHAALLLE-UHFFFAOYSA-N
Formula:	C4H3BrN2O2
SMILES:	O=c1[nH]cc(Br)c(=O)[nH]1
Mol. weight [g/mol]:	190.98
CAS:	51-20-7

Physical Properties

Property code	Value	Unit	Source
hsub	151.40 ± 2.50	kJ/mol	NIST Webbook
log10ws	0.08		Crippen Method
logp	-1.138		Crippen Method
mcvol	92.660	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	148.10	kJ/mol	409.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51207&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume