2,4(1H,3H)-PYRIMIDINEDITHIONE

Other names:	Uracil, 2,4-dithio-
	Dithiouracil
	2,4-Dimercaptopyrimidine
	2,4-Dithiouracil
	2,4-Dithioxopyrimidine
	2,4-Pyrimidinedithiol
	Pyrimidine-2,4-dithiol
	2,4-Dithiopyrimidine
	Dithiopyrimidine
	USAF CB-14
	NSC 42031
Inchi:	InChI=1S/C4H4N2S2/c7-3-1-2-5-4(8)6-3/h1-2H,(H2,5,6,7,8)
InchiKey:	ZEQIWKHCJWRNTH-UHFFFAOYSA-N
Formula:	C4H4N2S2
SMILES:	S=c1cc[nH]c(=S)[nH]1
Mol. weight [g/mol]:	144.22

Physical Properties

Property code	Value	Unit	Source
affp	911.40	kJ/mol	NIST Webbook
basg	880.50	kJ/mol	NIST Webbook
ea	1.40 ± 0.10	eV	NIST Webbook
ie	7.83	eV	Cheméo Relay (1.0)
log10ws	-2.51		Cheméo Relay (1.0)
logp	0.838		Crippen Method
mcvol	96.120	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	119.70 ± 2.40	kJ/mol	418.00	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=C2001936&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
ea:	Electron affinity
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