Propylthiouracil

Other names:	2,3-Dihydro-6-propyl-2-thioxo-4(1H)-pyrimidinone
	2-Mercapto-4-hydroxy-6-n-propylpyrimidine
	2-Mercapto-6-propyl-4-pyrimidone
	2-Mercapto-6-propylpyrimid-4-one
	2-Thio-4-oxo-6-propyl-1,3-pyrimidine
	2-Thio-6-propyl-1,3-pyrimidin-4-one
	4(1H)-Pyrimidinone, 2,3-dihydro-6-propyl-2-thioxo-
	4-Hydroxy-2-mercapto-6-propylpyrimidine
	6-Propil-tiouracile
	6-Propyl-2-thio-2,4(1H,3H)-pyrimidinedione
	6-Propyl-2-thiouracil
	6-Propylthiouracil
	6-Thio-4-propyluracil
	6-n-Propyl-2-thiouracil
	6-n-Propylthiouracil
	NSC 6498
	PTU
	PTU (thyreostatic)
	Procasil
	Propacil
	Propilthiouracil
	Propycil
	Propyl-Thiorist
	Propyl-Thyracil
	Propylthiorit
	Propythiouracil
	Prothiucil
	Prothiurone
	Prothycil
	Prothyran
	Protiural
	Tegretol
	Thiuragyl
	Thyreostat II
	Uracil, 6-propyl-2-thio-
Inchi:	InChI=1S/C7H10N2OS/c1-2-3-5-4-6(10)9-7(11)8-5/h4H,2-3H2,1H3,(H2,8,9,10,11)
InchiKey:	KNAHARQHSZJURB-UHFFFAOYSA-N
Formula:	C15H12N2O
SMILES:	CCCc1cc(=O)[nH]c(=S)[nH]1
Mol. weight [g/mol]:	236.27

CAS: 51-52-5

Physical Properties

Property code	Value	Unit	Source
ie	8.07 ± 0.08	eV	NIST Webbook
log10ws	-2.15		Aqueous Solubility Prediction Method
logp	0.421		Crippen Method
mcvol	127.910	ml/mol	McGowan Method
tf	492.82	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	1.03e-04	kPa	401.14	Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.
pvap	1.24e-04	kPa	403.18	Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.
pvap	1.51e-04	kPa	405.17	Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.
pvap	1.96e-04	kPa	407.15	Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.

pvap	2.31e-04	kPa	409.17	Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.
pvap	2.74e-04	kPa	411.16	Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.
pvap	3.32e-04	kPa	413.15	Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.
pvap	4.10e-04	kPa	415.17	Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.
pvap	4.84e-04	kPa	417.18	Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.
pvap	5.83e-04	kPa	419.15	Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.
pvap	7.14e-04	kPa	421.22	Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.
pvap	8.53e-04	kPa	423.21	Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51525&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility modelling and thermodynamic aspect of 2,3-dihydro-6-propyl-2-thioxo-4(1H)-pyrimidinone (propylthiouracil) in binary aqueous solutions of several alcohols:	https://www.doi.org/10.1016/j.jct.2018.12.038
Thermochemistry of 6-propyl-2-thiouracil: an experimental and computational study.	https://www.doi.org/10.1016/j.tca.2014.04.018
Prediction of Solubility in Aqueous Solutions of Ethylene Glycol, N,N-Dimethylformamide, N-Methyl-2-pyrrolidone, and Dimethylsulfoxide: Measurement and Thermodynamic Modeling:	https://www.doi.org/10.1021/acs.jced.9b00201
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tf:	Normal melting (fusion) point