

Tisopurine

Other names:	4H-Pyrazolo[3,4-d]pyrimidine-4-thione, 1,5-dihydro- Allopurinol, thio- MPP MPP (Pharmaceutical) Pyrazolo[3,4-d]Pyrimidine-4-thiol Thiopurinol 1H-Pyrazolo[3,4-d]pyrimidine-4-thiol 1H-Pyrazolo[3,4-d]pyrimidine-4(5H)-thione 4-Mercapto-1H-pyrazolo[3,4-d]pyrimidine 4-Mercaptopyrazolo[3,4-d]pyrimidine 5H-Pyrazolo[3,4-d]pyrimidine-4-thione DO 970 RS 570/T NSC 1392
Inchi:	InChI=1S/C5H4N4S/c10-5-3-1-8-9-4(3)6-2-7-5/h1-2H,(H2,6,7,8,9,10)
InchiKey:	PYAOPMWCFSVFOT-UHFFFAOYSA-N
Formula:	C5H4N4S
SMILES:	Sc1ncnc2[nH]ncc12
Mol. weight [g/mol]:	152.18
CAS:	5334-23-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	0.160		Crippen Method
mcvol	98.660	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5334236&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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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