



Formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>S

MW: 152.18

Salt: H<sub>2</sub>O

CAS: 6112-76-1

Smiles: c12c(nc[nH]2)[nH]cnc1=S

**THERAPEUTIC CATEGORY:** 6-Mercaptopurine is a widely used antileukemic agent that inhibits de novo purine synthesis through incorporation of thiopurine methyltransferase metabolites into DNA and RNA.

ACCEPTORS: 0

DONORS: 2

ROTATION BONDS: 0

N+O: 4

Chiral Centers: 0

LogP: 0.41

LogS: -2.57

LIPINSKI: 4

Synonyms:

1,7-dihydro-6h-purin-6-thion,monohydrat;1,7-dihydro-6h-purine-6-thionemonohydrate;1,7-dihydro-6h-purine-6-thionmonohydrate;6h-purin-6-thion,monohydrat;6-merkaptopurin,monohydrat;purin-6-thiol,monohydrat;PURINE-6-THIOL, MONOHYDRATE;MERCALEUKIN MONOHYDRATE

CAS:6112-76-1

MF:C5H6N4OS

MW:170.19

EINECS:212-968-3

Product Categories:Pyridines, Pyrimidines, Purines and Pteredines;Purine;Heterocyclic Compounds;Antitumors for Research and Experimental Use;Biochemistry;Nucleobases and their analogs;Nucleosides, Nucleotides & Related Reagents;Nucleic acids;Bases & Related Reagents;Heterocycles;Nucleotides;Sulfur & Selenium Compounds 6-Mercaptopurine monohydrate

Chemical Properties: mp >300 C(lit.) storage temp. Store at 0-5 solubility INSOLUBLE Water Solubility INSOLUBLE Merck 14,5871 BRN 4012091 Stability:Stable. Incompatible with strong oxidizing agents, acids, strong bases. Light sensitive.

CAS DataBase Reference: 6112-76-1(

CAS DataBase Reference: ) EPA Substance Registry System6H-Purine-6-thione, 1,7-dihydro-, monohydrate(6112-76-1) Xn,Xi Risk Statements 22-36/37/38-63-20/21/22 Safety Statements 22-36/37/39-45-36/37 WGK Germany 3 RTECS UP0400000 HS Code 29335995 6-Mercaptopurine monohydrate 6-Mercaptopurine monohydrate

Usage And Synthesis:

Chemical Properties: white to light yellow crystal powder UsageAn immunosuppressive drug used to treat leukemia. It is also used for pediatric non-Hodgkin lymphoma, polycythemia vera, and psoriatic arthritis General DescriptionOdorless light yellow to yellow crystalline powder. Becomes anhydrous at 284F. Air & Water Reactions6-Mercaptopurine monohydrate is sensitive to light and oxidation. Insoluble in water. Reactivity Profile6-Mercaptopurine monohydrate reacts with strong oxidizing agents, strong bases and strong acids. Fire HazardFlash point data for

6-Mercaptopurine monohydrate are not available. 6-Mercaptopurine monohydrate is probably combustible. 6-Mercaptopurine monohydrate

