

# Typical Product Specifications & Properties

## Thiothixene

CAS Number: : 22189-31-7

Specifications	Limits
SMILES	CN1CCN(CC1)CC/C=C\2/c3ccccc3Sc4c2cc(cc4)S(=O)(=O)N(C)C.O.O.Cl.Cl
InChI	MEUAAEMCZUPORO-LRSHZYOCSA-N
InChIKey	1S/C23H29N3O2S2.2ClH.2H2O/c1-24(2)30(27,28)18-10-11-23-21(17-18)19(20-7-4-5-9-22(20)29-23)8-6-12-26-15-13-25(3)14-16-26;;;/h4-5,7-11,17H,6,12-16H2,1-3H3;2*1H;2*1H2/b19-8-;;;
log P (octanol-water)	3.78
Atmospheric OH Rate Constant	2.92E-10 cm3/molecule-sec
Henry's Law Constant	3.70E-16 atm-m3/mole
Vapor Pressure	2.56E-12 mm Hg
Water solubility	0.764 mg/L