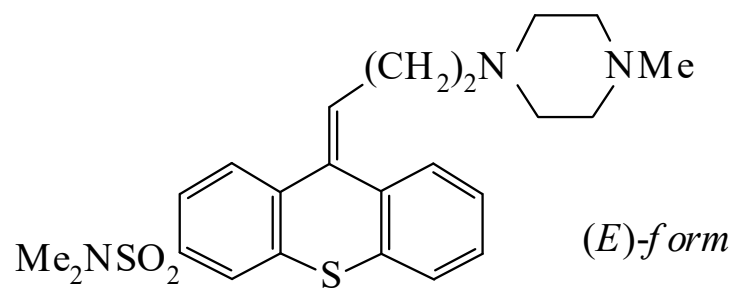




>>>Entry Name: Tiotixene, INN, JAN

Synonym(s): *N,N*-Dimethyl-9-[3-(4-methyl-1-piperazinyl)propylidene]-9*H*-thioxanthene-2-sulfonamide, 9Cl. **Thiothixene**, BAN, USAN. Navane. Navaron. NSC 108165. Orbinamon. P 4657B. CP 12252



CAS Registry Number: 5591-45-7

Related CAS Registry Numbers(s): 22189-31-7 49746-09-0

Molecular Formula: $\text{C}_{23}\text{H}_{29}\text{N}_3\text{O}_2\text{S}_2$

Molecular Weight: 443.633

Accurate Mass: 443.170117

Percentage Composition: C 62.27%; H 6.59%; N 9.47%; O 7.21%; S 14.46%

Use/Importance: Tranquilliser, neuroleptic agent

Calculated Log P Data: Log P 4.95 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 720 mg/kg. Human reprod. and exp. teratogenic effects

Sigma: T0780

>>>Variant: (*E*)-form

CAS Registry Number: 3313-27-7

Molecular Formula: $\text{C}_{23}\text{H}_{29}\text{N}_3\text{O}_2\text{S}_2$

Molecular Weight: 443.633

Accurate Mass: 443.170117

Percentage Composition: C 62.27%; H 6.59%; N 9.47%; O 7.21%; S 14.46%

Melting Point: Mp 123-124.5°

>>>Derivative: Dimaleate

Melting Point: Mp 158-160.5°

>>>Derivative: Dioxalate

Melting Point: Mp 229°

>>>Variant: (*Z*)-form

CAS Registry Number: 3313-26-6

Molecular Formula: $\text{C}_{23}\text{H}_{29}\text{N}_3\text{O}_2\text{S}_2$

Molecular Weight: 443.633

Accurate Mass: 443.170117

Percentage Composition: C 62.27%; H 6.59%; N 9.47%; O 7.21%; S 14.46%

Melting Point: Mp 147.5-149°

Other Data: Has greater pharmacological activity than E-form

>>>Derivative: Hydrochloride (1:2)

Synonym(s): **Thiothixene hydrochloride**, USAN

CAS Registry Number: 58513-59-0

Physical Description: Dihydrate

Hazard & Toxicity: LD₅₀ (rat, orl) 410 mg/kg

References: