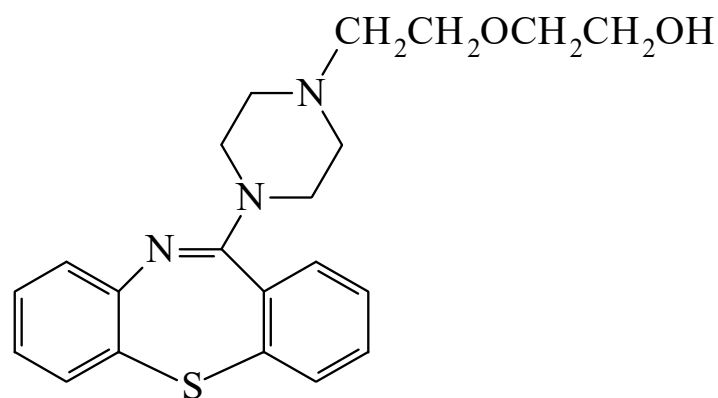




>>Entry Name: Quetiapine, BAN, INN

Synonym(s): 2-[2-(4-Dibenzo[*b,f*][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]ethanol, 9Cl. 11-[4-[2-(2-Hydroxyethoxy)ethyl]-1-piperazinyl]dibenzo[*b,f*][1,4]thiazepine. Seroquel. Z 204636



CAS Registry Number: 111974-69-7

Molecular Formula: C₂₁H₂₅N₃O₂S

Molecular Weight: 383.513

Accurate Mass: 383.166747

Percentage Composition: C 65.77%; H 6.57%; N 10.96%; O 8.34%; S 8.36%

Biological Use/Importance: Antipsychotic and neuroleptic agent

Development Status: Marketed drug. Approved for clinical use by FDA (1997) in Switzerland and Finland (1999)

Calculated Log P Data: Log P 3.51 (uncertain value) (calc)

>>Derivative: Hydrochloride (1:2)

CAS Registry Number: 111997-26-3

Physical Description: Cryst.

Melting Point: Mp 218-219°

>>Derivative: Fumarate (2:1)

CAS Registry Number: 111974-72-2

Physical Description: Cryst.

Melting Point: Mp 172-173°

>>Derivative: Maleate

CAS Registry Number: 111974-71-1

Physical Description: Cryst.

Melting Point: Mp 129-130°

References:

- Eur. Pat.*, 1987, *ICI Americas*, 240 228; *CA*, **108**, 37876q, (*synth, pharmacol*)
Campbell, A. *et al.*, *Psychopharmacology (Berlin)*, 1991, **103**, 323, (*pharmacol*)
Pullen, R.H. *et al.*, *J. Chromatogr.*, 1992, **573**, 49, (*hplc, gc-ms*)
Saller, C.F. *et al.*, *Psychopharmacology (Berlin)*, 1993, **112**, 285; 293; 299, (*pharmacol*)
Goldstein, J.M., *Drugs of Today (Barcelona)*, 1999, **35**, 193-210