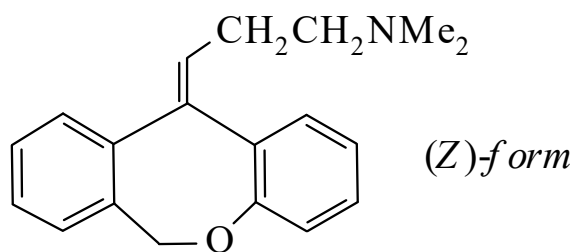




>>>Entry Name: **Doxepin**, BAN, INN

Synonym(s): 3-Dibenz[*b,e*]oxepin-11-(6*H*)-ylidene-*N,N*-dimethyl-1-propanamine, 9Cl. 11-(3-Dimethylaminopropylidene)-6*H*-dibenz[*b,e*]oxepin



CAS Registry Number: 1668-19-5

Related CAS Registry Numbers(s): 3607-34-9 4698-39-9

Type of Compound Code(s): XA1450 XA4510

Molecular Formula: C₁₉H₂₁NO

Molecular Weight: 279.381

Accurate Mass: 279.162314

Percentage Composition: C 81.68%; H 7.58%; N 5.01%; O 5.73%

General Statement: The pharmaceutical prod. is a mixt. of (*E*)- and (*Z*)-isomers (approx. ratio 5:1 in the case of the coml. hydrochloride)

Use/Importance: Histamine H₁- and H₂-receptor antagonist. Antidepressant, sedative, antipruritic

Physical Description: Oil

Boiling Point: Bp_{0.03} 154-157°

Calculated Log P Data: Log P 3.96 (uncertain value) (calc)

Other Data: (*E*)-form metab. to (*Z*)-form *in vivo*. Analogue of Dosulepin [FWK01-X](#)

>>>Derivative: Hydrochloride

Synonym(s): **Doxepin hydrochloride**, USAN. Adapin. Curatin. Sinequan. NSC 108160. Many other names

CAS Registry Number: 1229-29-4

Melting Point: Mp 188-189° (184-186°)

Hazard & Toxicity: LD₅₀ (rat, orl) 147 mg/kg. Exp. reprod. and teratogenic effects

Sigma: D0928

>>>Derivative: *N*-De-Me

Synonym(s): Desmethyldoxepin

CAS Registry Number: 1225-56-5

Extra CAS Registry Numbers(s): 58534-46-6 67035-76-1

Molecular Formula: C₁₈H₁₉NO

Molecular Weight: 265.354

Accurate Mass: 265.146664

Percentage Composition: C 81.48%; H 7.22%; N 5.28%; O 6.03%

Use/Importance: Pharmacologically active human metabolite of doxepin

Melting Point: Mp 60-62°

Boiling Point: Bp_{0.01} 158-165°

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

Synonym(s): **Cidoxepin**, INN

CAS Registry Number: 3607-18-9

Molecular Formula: C₁₉H₂₁NO

Molecular Weight: 279.381

Accurate Mass: 279.162314

Percentage Composition: C 81.68%; H 7.58%; N 5.01%; O 5.73%

Development Status: Never marketed

>>>Derivative: Hydrochloride

Synonym(s): **Cidoxepin hydrochloride**, USAN. P 4599

CAS Registry Number: 25127-31-5

Physical Description: Cryst. (CHCl₃/CCl₄)

Melting Point: Mp 211.5-212°

References: