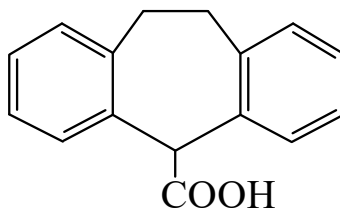




>>Entry Name: 10,11-Dihydro-5*H*-dibenzo[*a,d*]cycloheptene-5-carboxylic acid, 9Cl, 8Cl

Synonym(s): Dibenzo[*a,d*]cycloheptadiene-5-carboxylic acid. 5*H*-Dibenzo[*a,d*]cycloheptane-5-carboxylic acid. Suberane-5-carboxylic acid



CAS Registry Number: 5018-91-7

Molecular Formula: C₁₆H₁₄O₂

Molecular Weight: 238.285

Accurate Mass: 238.09938

Percentage Composition: C 80.65%; H 5.92%; O 13.43%

Physical Description: Needles (CH₂Cl₂)

Melting Point: Mp 237-238°

>>Derivative: Amide

Synonym(s): Cyheptamide, INN, USAN. AY 8682. BS 7029. ICI 51426

CAS Registry Number: 7199-29-3

Molecular Formula: C₁₆H₁₅NO

Molecular Weight: 237.301

Accurate Mass: 237.115364

Percentage Composition: C 80.98%; H 6.37%; N 5.90%; O 6.74%

Use/Importance: Anticonvulsant

Physical Description: Long needles (MeCN)

Melting Point: Mp 193-194°

Calculated Log P Data: Log P 2.5 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 2400 mg/kg

Sigma: C4080

>>Derivative: Chloride

Molecular Formula: C₁₆H₁₃ClO

Molecular Weight: 256.731

Accurate Mass: 256.065492

Percentage Composition: C 74.86%; H 5.10%; Cl 13.81%; O 6.23%

Melting Point: Mp 71-72°

>>Derivative: Tropine ester

Synonym(s): Cyheptropine, INN. 8-Methyl-8-azabicyclo[3.2.1]oct-3-yl 10,11-dihydro-5*H*-dibenzo[*a,d*]cycloheptene-5-carboxylate. BS 7042

CAS Registry Number: 602-40-4

Molecular Formula: C₂₄H₂₇NO₂

Molecular Weight: 361.483

Accurate Mass: 361.204179

Percentage Composition: C 79.74%; H 7.53%; N 3.87%; O 8.85%

Use/Importance: Antiarrhythmic agent

Development Status: Never marketed

Calculated Log P Data: Log P 4.25 (calc)

>>Derivative: Tropine ester; hydrochloride

CAS Registry Number: 10123-16-7

Melting Point: Mp 272-275°

>>Derivative: Tropine ester, maleate

Melting Point: Mp 175-177°

References: