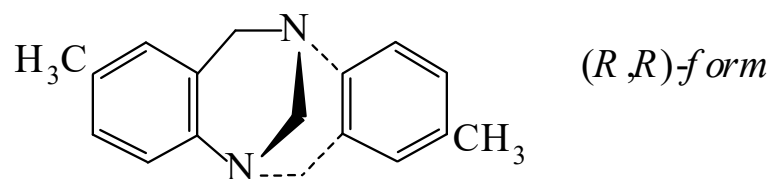




>>Entry Name: Troeger's base

Synonym(s): 2,8-Dimethyl-6*H*,12*H*-5,11-methanodibenzo[*b,f*][1,5]diazocine, 9Cl



CAS Registry Number: 529-81-7

Molecular Formula: C₁₇H₁₈N₂

Molecular Weight: 250.343

Accurate Mass: 250.146998

Percentage Composition: C 81.56%; H 7.25%; N 11.19%

Rare Chemicals Library: S44142-2

>>Variant: (*R,R*)-form

CAS Registry Number: 14645-24-0

Molecular Formula: C₁₇H₁₈N₂

Molecular Weight: 250.343

Accurate Mass: 250.146998

Percentage Composition: C 81.56%; H 7.25%; N 11.19%

Physical Description: Prisms

Melting Point: Mp 127-128°

Optical Rotation: [α]_D¹⁶ -272 (c, 0.275 in hexane)

Other Data: Incorr. abs. config. prev. assigned

Aldrich: 37465-2

Fluka: 40765

>>Variant: (*S,S*)-form

CAS Registry Number: 21451-74-1

Molecular Formula: C₁₇H₁₈N₂

Molecular Weight: 250.343

Accurate Mass: 250.146998

Percentage Composition: C 81.56%; H 7.25%; N 11.19%

Physical Description: Prisms (petrol)

Melting Point: Mp 26-27.5°

Optical Rotation: [α]_D¹⁷ +285 (c, 0.289 in hexane). [α]_D²⁰ +310 (c, 0.298 in CHCl₃)

Aldrich: 37464-4

Fluka: 40764

>>Variant: ($\pm$)-form

CAS Registry Number: 72151-03-2

Molecular Formula: C₁₇H₁₈N₂

Molecular Weight: 250.343

Accurate Mass: 250.146998

Percentage Composition: C 81.56%; H 7.25%; N 11.19%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 135-136°

Other Data: Resolvable chromatographically. Forms clathrates

Aldrich: 13222-5

>>Derivative: Hydrochloride

Melting Point: Mp 213°

>>Derivative: Picrate

Melting Point: Mp 188-189°

References: