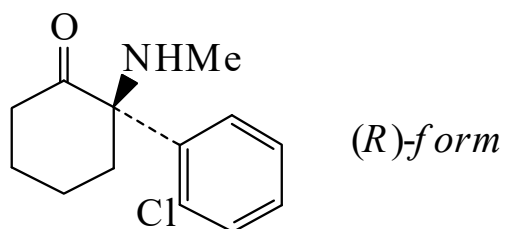




>>Entry Name: Ketamine, BAN

Synonym(s): 2-(2-Chlorophenyl)-2-(methylamino)cyclohexanone, 9Cl, 8Cl



CAS Registry Number: 100477-72-3

Related CAS Registry Numbers(s): 33643-47-9 100477-73-4

Molecular Formula: C₁₃H₁₆ClNO

Molecular Weight: 237.728

Accurate Mass: 237.092041

Percentage Composition: C 65.68%; H 6.78%; Cl 14.91%; N 5.89%; O 6.73%

Use/Importance: Anaesthetic

Calculated Log P Data: Log P 2.93 (calc)

Other Data: Abs config. prev. descr. incorr. as (S)-(+); in 1991 this was revised to S-(−) (Ratti-Moberg *et al*)

>>Variant: (R)-form

Synonym(s): (+)-form

CAS Registry Number: 33643-49-1

Molecular Formula: C₁₃H₁₆ClNO

Molecular Weight: 237.728

Accurate Mass: 237.092041

Percentage Composition: C 65.68%; H 6.78%; Cl 14.91%; N 5.89%; O 6.73%

>>Variant: (S)-form

Synonym(s): Esketamine, BAN, INN

CAS Registry Number: 33643-46-8

Molecular Formula: C₁₃H₁₆ClNO

Molecular Weight: 237.728

Accurate Mass: 237.092041

Percentage Composition: C 65.68%; H 6.78%; Cl 14.91%; N 5.89%; O 6.73%

Other Data: Pharmacol. active isomer

>>Derivative: Hydrochloride

Synonym(s): Vetalar

CAS Registry Number: 33795-24-3

Optical Rotation: $[\alpha]_D^{25} +91.2$ (c, 0.3 in H₂O)

Sigma: K1884

>>Variant: (±)-form

CAS Registry Number: 6740-88-1

Molecular Formula: C₁₃H₁₆ClNO

Molecular Weight: 237.728

Accurate Mass: 237.092041

Percentage Composition: C 65.68%; H 6.78%; Cl 14.91%; N 5.89%; O 6.73%

Physical Description: Cryst. (pentane/Et₂O)

Melting Point: Mp 92-93°

Hazard & Toxicity: LD₅₀ (mus, ipr) 400 mg/kg. Exp. teratogen

>>Derivative: Hydrochloride

Synonym(s): Ketamine hydrochloride, JAN, USAN. Ketalar. Ketaset. Vetalar. CI 581. CL 369. CM 52372-2. Many other names

CAS Registry Number: 1867-66-9

Hazard & Toxicity: Can cause hallucinations and psychoses esp. if abused. Other emergence reactions reported from anaesthetic uses. LD₅₀ (mus, ipr) 224 mg/kg. Exp. teratogen

Aldrich: 34309-9

Sigma: K2753