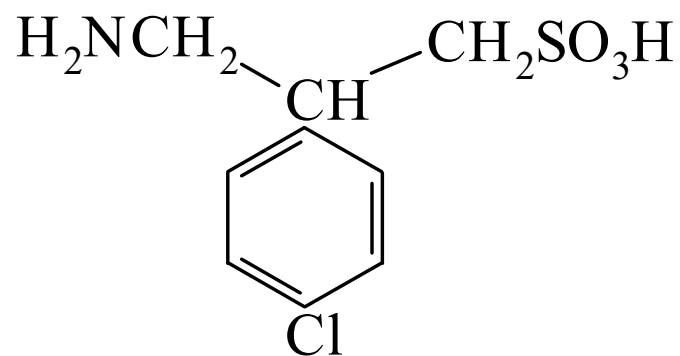




>>Entry Name: 3-Amino-2-(4-chlorophenyl)-1-propanesulfonic acid

Synonym(s): β -(Aminomethyl)-4-chlorobenzeneethanesulfonic acid, 9Cl. Saclofen



CAS Registry Number: 125464-42-8

Molecular Formula: $C_9H_{12}ClNO_3S$

Molecular Weight: 249.717

Accurate Mass: 249.022641

Percentage Composition: C 43.29%; H 4.84%; Cl 14.20%; N 5.61%; O 19.22%; S 12.84%

Use/Importance: GABA_B receptor antagonist. Pharmacological tool

Calculated Log P Data: Log P -2.32 (uncertain value) (calc)

Sigma: A3441

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

CAS Registry Number: 134589-60-9

Molecular Formula: $C_9H_{12}ClNO_3S$

Molecular Weight: 249.717

Accurate Mass: 249.022641

Percentage Composition: C 43.29%; H 4.84%; Cl 14.20%; N 5.61%; O 19.22%; S 12.84%

Physical Description: Solid

Melting Point: Mp 320°

>>Derivative: Hydrochloride

CAS Registry Number: 127876-35-1

Physical Description: Cryst. (H₂O)

Melting Point: Mp 310-315 dec.°

References:

Kerr, D.I.B. *et al.*, *Neurosci. Lett.*, 1989, **107**, 239; 1990, **113**, 107, (*pharmacol*)

Abbenante, G. *et al.*, *Aust. J. Chem.*, 1990, **43**, 213; 1992, **45**, 1801, (*synth, pmr, cmr*)

Li, C.-S. *et al.*, *Synthesis*, 1991, 244, (*synth, pmr, ms*)