



Formula: C₁₀H₁₂ClNO₂

MW: 213.66

CAS: 1334-47-0

MDL NUMBER: MFCD00055143

IUPAC: 4-amino-3-(4-chlorophenyl)butanoic acid

Smiles: C(CC(c1ccc(Cl)cc1)CN)(=O)O

THERAPEUTIC CATEGORY: Muscle Relaxant, Antispastic Agent

ACCEPTORS: 2

DONORS: 3

ROTATION BONDS: 4

N+O: 3

Chiral Centers: 1

LogP: 1.78

LogS: -3.19

LIPINSKI: 4

Monograph Number: 0000939

Title: Baclofen

CAS Registry Number: 1134-47-0

CAS Name: b-(Aminomethyl)-4-chlorobenzenepropanoic acid

Additional Names: b-(aminomethyl)-p-chlorohydrocinnamic acid;
g-amino-b-(p-chlorophenyl)butyric acid; b-(4-chlorophenyl)GABA

Manufacturers' Codes: Ba-34647

Trademarks: Baclon (Leiras); Clofen (Alphapharm); Lioresal (Novartis)

Molecular Formula: C₁₀H₁₂ClNO₂

Molecular Weight: 213.66.

Percent Composition: C 56.21%, H 5.66%, Cl 16.59%, N 6.56%, O 14.98%

Literature References: Specific GABA-B receptor agonist. Prepn: NL 6407755; H. Keberle et al., US 3471548 (1965, 1969 both to Ciba). Toxicity study: T. Tadokoro et al., Osaka Daigaku Igaku Zasshi 28, 265 (1976), C.A. 88, 183016u (1978). Comprehensive description: S. Ahuja, Anal. Profiles Drug Subs. 14, 527-548 (1985). Review of pharmacology and therapeutic efficacy in spasticity: R. N. Brogden et al., Drugs 8, 1-14 (1974); of intrathecal use in spinal cord injury: K. S. Lewis, W. M. Mueller, Ann. Pharmacother. 27, 767-774 (1993). Clinical evaluation in reflex sympathetic dystrophy: B. J. van Hilten et al., N. Engl. J. Med. 343, 625 (2000).

Properties: Crystals from water, mp 206-208 (Keberle); 189-191, (Uchimaru). LD₅₀ in male mice, rats (mg/kg): 45, 78 i.v.; 103, 115 s.c.; 200, 145 orally (Tadokoro).

Melting point: mp 206-208 (Keberle); 189-191, (Uchimaru)

Toxicity data: LD₅₀ in male mice, rats (mg/kg): 45, 78 i.v.; 103, 115 s.c.; 200, 145 orally (Tadokoro)

Derivative Type: Hydrochloride

Molecular Formula: C₁₀H₁₃Cl₂NO₂

Molecular Weight: 250.12.

Percent Composition: C 48.02%, H 5.24%, Cl 28.35%, N 5.60%, O 12.79%

Properties: mp 179-181.

Melting point: mp 179-181

Therap-Cat: Muscle relaxant (skeletal).

Synonyms: Baclofen(Rs)-

CAS:

MF:

MW:0

EINECS:

Product Categories: Baclofen(Rs)- Baclofen(Rs)-

Usage And Synthesis: Baclofen(Rs)-

