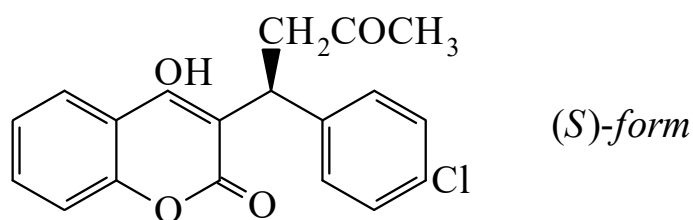




>>Entry Name: Coumachlor, BSI, ISO

Synonym(s): 3-[1-(4-Chlorophenyl)-3-oxobutyl]-4-hydroxy-2H-1-benzopyran-2-one, 9Cl. 3-[1-(4-Chlorophenyl)-3-oxobutyl]-4-hydroxycoumarin. Tomorin. Ratilan. Cumachlor. Chlorowarfarin



CAS Registry Number: 81-82-3

Related CAS Registry Numbers(s): 95041-39-7 95271-89-9

Molecular Formula: C₁₉H₁₅ClO₄

Molecular Weight: 342.778

Accurate Mass: 342.065887

Percentage Composition: C 66.58%; H 4.41%; Cl 10.34%; O 18.67%

Aldrich: 18921-9

Sigma: A2029

>>Variant: (S)-form

CAS Registry Number: 70888-76-5

Molecular Formula: C₁₉H₁₅ClO₄

Molecular Weight: 342.778

Accurate Mass: 342.065887

Percentage Composition: C 66.58%; H 4.41%; Cl 10.34%; O 18.67%

Melting Point: Mp 103-106°

>>Variant: (±)-form

Molecular Formula: C₁₉H₁₅ClO₄

Molecular Weight: 342.778

Accurate Mass: 342.065887

Percentage Composition: C 66.58%; H 4.41%; Cl 10.34%; O 18.67%

Use/Importance: Rodenticide. Internal standard used in the analysis of Warfarin [CNP01-E](#). Commercially available

Physical Description: Cryst.

Melting Point: Mp 169-171°

Hazard & Toxicity: LD₅₀ (rat, orl) 187 mg/kg

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **2**, 329B, (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 313D, (*nmr*)
U.K. Pat., 1950, 701 111; *CA*, **49**, 2522d
Wheeler, C.R. *et al.*, *J. Med. Chem.*, 1979, **22**, 1122, (*synth, ir, pmr*)
Jeyaraj, G.L. *et al.*, *J. Chromatogr.*, 1984, **315**, 378, (*resoln*)
Pesticide Manual, 9th edn., 1991, No. 3320
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A97