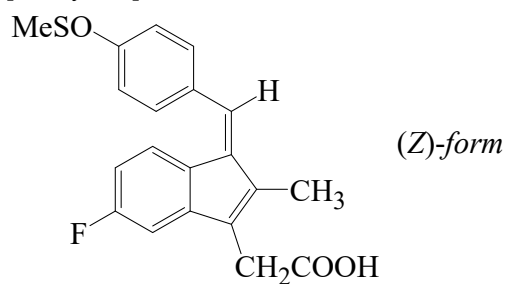




>>Entry Name: Sulindac, BAN, INN, JAN, USAN

Synonym(s): 5-Fluoro-2-methyl-1-[[4-(methylsulfinyl)phenyl]methylene]-1*H*-indene-3-acetic acid, 9Cl. Clinoril. Many other names



Molecular Formula: C₂₀H₁₇FO₃S

Molecular Weight: 356.417

Accurate Mass: 356.088243

Percentage Composition: C 67.40%; H 4.81%; F 5.33%; O 13.47%; S 9.00%

Use/Importance: Antiinflammatory, analgesic, antipyretic

Calculated Log P Data: Log P 2.77 (calc)

>>Variant: (*E*)-form

CAS Registry Number: 61812-46-2

Molecular Formula: C₂₀H₁₇FO₃S

Molecular Weight: 356.417

Accurate Mass: 356.088243

Percentage Composition: C 67.40%; H 4.81%; F 5.33%; O 13.47%; S 9.00%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 178-181°

>>Derivative: Deoxy

Synonym(s): 5-Fluoro-2-methyl-1-[[4-(methylthio)phenyl]methylene]-1*H*-indene-3-acetic acid, 9Cl

CAS Registry Number: 61812-45-1

Extra CAS Registry Numbers(s): 32004-67-4

Molecular Formula: C₂₀H₁₇FO₂S

Molecular Weight: 340.418

Accurate Mass: 340.093328

Percentage Composition: C 70.57%; H 5.03%; F 5.58%; O 9.40%; S 9.42%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 188-191°

>>Variant: (*Z*)-form

CAS Registry Number: 38194-50-2

Molecular Formula: C₂₀H₁₇FO₃S

Molecular Weight: 356.417

Accurate Mass: 356.088243

Percentage Composition: C 67.40%; H 4.81%; F 5.33%; O 13.47%; S 9.00%

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 187-188 dec.°

Solubility: Sol. dil. acids, alkalis

pKa Value: p*K*_a 4.5

Other Data: Mod. unstable in air. The pharmacol. prod. is probably the (*Z*)-form

Hazard & Toxicity: LD₅₀ (rat, orl) 264 mg/kg

Sigma: S8139

>>Derivative: Deoxy

CAS Registry Number: 49627-27-2

Extra CAS Registry Numbers(s): 32004-67-4

Melting Point: Mp 190-193°