



>>Entry Name: 9-Anthracenecarboxylic acid, 9Cl

Synonym(s): *ms*-Anthracenecarboxylic acid. *ms*-Anthroic acid. Anthroic acid

CAS Registry Number: 723-62-6

Molecular Formula: C₁₅H₁₀O₂

Molecular Weight: 222.243

Accurate Mass: 222.06808

Percentage Composition: C 81.07%; H 4.54%; O 14.40%

Biological Use/Importance: Chloride channel blocker

Physical Description: Pale yellow needles (EtOH)

Melting Point: Mp 207 dec.°

pKa Value: pK_a 3.66 (20°)

Hazard & Toxicity: LD₅₀ (mus, ipr) 750 mg/kg

Aldrich: A8940-5

Fluka: 10605

Rare Chemicals Library: S5906-5

Sigma: A4678

>>Derivative: Me ester

CAS Registry Number: 1504-39-8

Molecular Formula: C₁₆H₁₂O₂

Molecular Weight: 236.27

Accurate Mass: 236.08373

Percentage Composition: C 81.34%; H 5.12%; O 13.54%

Physical Description: Yellow prisms

Melting Point: Mp 111°

Rare Chemicals Library: S85281-3

>>Derivative: Amide

CAS Registry Number: 34810-13-4

Molecular Formula: C₁₅H₁₁NO

Molecular Weight: 221.258

Accurate Mass: 221.084064

Percentage Composition: C 81.43%; H 5.01%; N 6.33%; O 7.23%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 219-219.5°

Aldrich: 30161-2

>>Derivative: Chloride

Synonym(s): 9-Anthracenecarbonyl chloride, 9Cl. 9-Anthroyl chloride, 8Cl

CAS Registry Number: 16331-52-5

Use/Importance: Hplc derivatising agent for hydroxy compds.

Physical Description: Dull yellow solid

Melting Point: Mp 93.5-94.5°

>>Derivative: Nitrile

Synonym(s): 9-Cyanoanthracene

CAS Registry Number: 1210-12-4

Molecular Formula: C₁₅H₉N

Molecular Weight: 203.243

Accurate Mass: 203.073499

Percentage Composition: C 88.65%; H 4.46%; N 6.89%

Melting Point: Mp 173-177°

Aldrich: 15276-5

Rare Chemicals Library: S11435-9