



>>Entry Name: 2-Naphthalenecarboxylic acid, 9CI

Synonym(s): 2-Naphthoic acid

CAS Registry Number: 93-09-4

Extra CAS Registry Numbers(s): 1320-04-3

Molecular Formula: C₁₁H₈O₂

Molecular Weight: 172.183

Accurate Mass: 172.05243

Percentage Composition: C 76.73%; H 4.68%; O 18.58%

Physical Description: Needles (petrol) or plates (Me₂CO)

Melting Point: Mp 185.5°

pKa Value: pK_a 4.17 (4.28)

Hazard & Toxicity: Skin and mucous membrane irritant. LD₅₀ (rat, orl) 4500 mg/kg

Aldrich: 18024-6

Fluka: 70400

Rare Chemicals Library: S56195-9

Sigma: N0259

>>Derivative: Me ester

CAS Registry Number: 2459-25-8

Molecular Formula: C₁₂H₁₀O₂

Molecular Weight: 186.21

Accurate Mass: 186.06808

Percentage Composition: C 77.40%; H 5.41%; O 17.18%

Melting Point: Mp 77°

Boiling Point: Bp 290°

Aldrich: 44907-5

Rare Chemicals Library: S5787-9

>>Derivative: Et ester

CAS Registry Number: 3007-91-8

Molecular Formula: C₁₃H₁₂O₂

Molecular Weight: 200.237

Accurate Mass: 200.08373

Percentage Composition: C 77.98%; H 6.04%; O 15.98%

Melting Point: Mp 77°

Boiling Point: Bp₇₄ 224°

Rare Chemicals Library: S32913-4

>>Derivative: Benzyl ester

CAS Registry Number: 53531-11-6

Molecular Formula: C₁₈H₁₄O₂

Molecular Weight: 262.307

Accurate Mass: 262.09938

Percentage Composition: C 82.42%; H 5.38%; O 12.20%

Physical Description: Cryst. (Et₂O/petrol)

Melting Point: Mp 63.5-64°

>>Derivative: Ph ester

CAS Registry Number: 82408-29-5

Molecular Formula: C₁₇H₁₂O₂

Molecular Weight: 248.281

Accurate Mass: 248.08373

Percentage Composition: C 82.24%; H 4.87%; O 12.89%

Melting Point: Mp 95-96°

>>Derivative: Fluoride