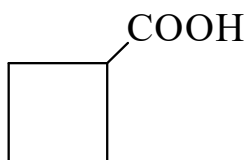




>>Entry Name: Cyclobutanecarboxylic acid, 9CI



CAS Registry Number: 3721-95-7

Molecular Formula: C₅H₈O₂

Molecular Weight: 100.117

Accurate Mass: 100.05243

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Physical Description: Liq.

Boiling Point: Bp 195°. Bp₁₅ 96°

pKa Value: pK_a 4.79 (25°,H₂O)

Refractive Index: n_D²⁰ 1.4433

Hazard & Toxicity: LD₅₀ (mus, ipr) 1270 mg/kg

Aldrich: C9560-9

Fluka: 28661

>>Derivative: Me ester

CAS Registry Number: 765-85-5

Molecular Formula: C₆H₁₀O₂

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Physical Description: Liq.

Boiling Point: Bp 136-136.5°

Rare Chemicals Library: S85195-7

>>Derivative: Et ester

CAS Registry Number: 14924-53-9

Molecular Formula: C₇H₁₂O₂

Molecular Weight: 128.171

Accurate Mass: 128.08373

Percentage Composition: C 65.60%; H 9.44%; O 24.97%

Physical Description: Liq.

Boiling Point: Bp 151.5-152°

Aldrich: 11386-7

Fluka: 28665

>>Derivative: Chloride

CAS Registry Number: 5006-22-4

Molecular Formula: C₅H₇ClO

Molecular Weight: 118.562

Accurate Mass: 118.018542

Percentage Composition: C 50.65%; H 5.95%; Cl 29.90%; O 13.49%

Physical Description: Liq.

Boiling Point: Bp 142-143°

Aldrich: C9570-6

>>Derivative: Amide

CAS Registry Number: 1503-98-6

Molecular Formula: C₅H₉NO

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

Physical Description: Flakes (Et₂O/EtOH)

Melting Point: Mp 152-153°

Rare Chemicals Library: S68074-5