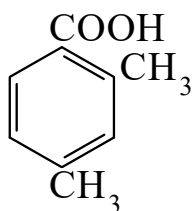




>>Entry Name: 2,4-Dimethylbenzoic acid, 9CI, 8CI

Synonym(s): *unsym-m*-Xylylic acid



CAS Registry Number: 611-01-8

Molecular Formula: C₉H₁₀O₂

Molecular Weight: 150.177

Accurate Mass: 150.06808

Percentage Composition: C 71.98%; H 6.71%; O 21.31%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 126-127°

Boiling Point: Bp₇₂₇ 267°

pKa Value: pK_{a1} 4.22 (25°)

Other Data: Sublimes

Aldrich: 13816-9

Fluka: 39582

>>Derivative: Me ester

CAS Registry Number: 23617-71-2

Molecular Formula: C₁₀H₁₂O₂

Molecular Weight: 164.204

Accurate Mass: 164.08373

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Physical Description: Oil

Melting Point: Mp -2°

Boiling Point: Bp 232-233°

>>Derivative: Et ester

CAS Registry Number: 33499-42-2

Molecular Formula: C₁₁H₁₄O₂

Molecular Weight: 178.23

Accurate Mass: 178.09938

Percentage Composition: C 74.13%; H 7.92%; O 17.95%

Physical Description: Oil

Boiling Point: Bp₄₀ 156°

>>Derivative: Chloride

CAS Registry Number: 21900-42-5

Molecular Formula: C₉H₉ClO

Molecular Weight: 168.622

Accurate Mass: 168.034192

Percentage Composition: C 64.11%; H 5.38%; Cl 21.02%; O 9.49%

Physical Description: Cryst.

Melting Point: Mp 25.5°

Boiling Point: Bp 234-236°. Bp₁₅ 113-115°

>>Derivative: Amide

CAS Registry Number: 73258-94-3

Molecular Formula: C₉H₁₁NO

Molecular Weight: 149.192

Accurate Mass: 149.084064

Percentage Composition: C 72.46%; H 7.43%; N 9.39%; O 10.72%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 179-181°