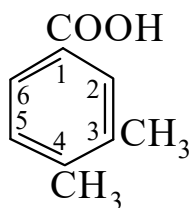




>>Entry Name: 3,4-Dimethylbenzoic acid, 9CI, 8CI

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



CAS Registry Number: 619-04-5

Type of Compound Code(s): VG0040

Molecular Formula: C₉H₁₀O₂

Molecular Weight: 150.177

Accurate Mass: 150.06808

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

Biological Source: Isol. from *Eryngium foetidum*

Physical Description: Prisms

Melting Point: Mp 166°

pKa Value: pK_a 4.5 (25°)

Other Data: Sublimes

Aldrich: D14940-3

Fluka: 39590

>>Derivative: Me ester

CAS Registry Number: 38404-42-1

Molecular Formula: C₁₀H₁₂O₂

Molecular Weight: 164.204

Accurate Mass: 164.08373

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

Physical Description: Liq.

Boiling Point: Bp₃₈ 132°

>>Derivative: Chloride

CAS Registry Number: 21900-23-2

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: Liq.

Boiling Point: Bp₁₀ 122°

>>Derivative: Amide

CAS Registry Number: 5580-33-6

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 131° (113-114°)

>>Derivative: Nitrile

Synonym(s): 3,4-Dimethylbenzonitrile. 4-Cyano-1,2-dimethylbenzene

CAS Registry Number: 22884-95-3

Molecular Formula: C₉H₉N

Molecular Weight: 131.177

Accurate Mass: 131.073499

Percentage Composition: C 82.41%; H 6.92%; N 10.68%

Physical Description: Cryst.

Melting Point: Mp 66°

Boiling Point: Bp 231-232°

Rare Chemicals Library: S45400-1