



>>Entry Name: **3,5-Dimethylbenzoic acid**, 9Cl, 8Cl

Synonym(s): *sym-m*-Xylylic acid. Mesitylenic acid

CAS Registry Number: 499-06-9

Structure by analogy with 2,3-Dimethylbenzoic acid, [DZV67-X](#)

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 or H₂O)

Melting Point: Mp 170°

pKa Value: pK_a 4.3

Other Data: Steam-volatile

Hazard & Toxicity: Explosions have occurred during prepn. by oxidn. of 1,3,5-Trimethylbenzene [BLP90-F](#) under pressure. Eye, skin and respiratory tract irritant

Aldrich: D14960-8

Fluka: 39600

>>Derivative: Me ester

CAS Registry Number: 25081-39-4

Molecular Formula: C₁₀H₁₂O₂

Molecular Weight: 164.204

Accurate Mass: 164.08373

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

Melting Point: Mp 35-36°

Boiling Point: Bp 239-240°

Aldrich: 37021-5

Rare Chemicals Library: S11219-4

>>Derivative: Et ester

CAS Registry Number: 21239-29-2

Molecular Formula: C₁₁H₁₄O₂

Molecular Weight: 178.23

Accurate Mass: 178.09938

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

Physical Description: Liq.

Boiling Point: Bp 241°. Bp₂ 74-75°

>>Derivative: Chloride

CAS Registry Number: 6613-44-1

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 109.5°

>>Derivative: Amide

CAS Registry Number: 5692-35-3

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 133°