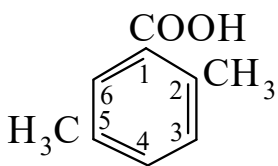




>>Entry Name: 2,5-Dimethylbenzoic acid, 9Cl, 8Cl

Synonym(s): *p*-Xylylic acid



CAS Registry Number: 610-72-0

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 *Ocinum gratissimum*

Physical Description: Needles (EtOH)

Melting Point: Mp 132°

Boiling Point: Bp 268°

pKa Value: pK_{a1} 4 (25°)

Other Data: Steam-volatile

Aldrich: 13817-7

Fluka: 39583

>>Derivative: Amide

CAS Registry Number: 5692-34-2

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.

Melting Point: Mp 186°

>>Derivative: Nitrile

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

CAS Registry Number: 13730-09-1

Molecular Formula: C₉H₉N

Molecular Weight: 131.177

Accurate Mass: 131.073499

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

Physical Description: Liq.

Boiling Point: Bp₇₃₀ 223-226°

Other Data: Steam-volatile

Rare Chemicals Library: S43334-9

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1102A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 209B; 455D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1330A; 1417A, (*ir*)

Schmid, A. *et al.*, *Ber.*, 1906, **39**, 938, (*synth*)

Nightingale, D.V. *et al.*, *J.O.C.*, 1953, **18**, 1529, (*synth*)

Qudrat-i-Khuda, M. *et al.*, *CA*, 1965, **62**, 811g, (*isol*)