



>>Entry Name: 3,5-Dibromo-4-methylbenzoic acid

Synonym(s): 3,5-Dibromo-*p*-toluic acid

CAS Registry Number: 67973-32-4

Molecular Formula: C₈H₆Br₂O₂

Molecular Weight: 293.942

Accurate Mass: 291.913452

Percentage Composition: C 32.69%; H 2.06%; Br 54.37%; O 10.89%

Physical Description: Needles (EtOH)

Melting Point: Mp 235-236°

>>Derivative: Me ester

CAS Registry Number: 74896-66-5

Molecular Formula: C₉H₈Br₂O₂

Molecular Weight: 307.969

Accurate Mass: 305.929102

Percentage Composition: C 35.10%; H 2.62%; Br 51.89%; O 10.39%

Melting Point: Mp 48°

Aldrich: 30105-1

>>Derivative: Et ester

Molecular Formula: C₁₀H₁₀Br₂O₂

Molecular Weight: 321.996

Accurate Mass: 319.944752

Percentage Composition: C 37.30%; H 3.13%; Br 49.63%; O 9.94%

Physical Description: Needles

Melting Point: Mp 80°

>>Derivative: Chloride

Molecular Formula: C₈H₅Br₂ClO

Molecular Weight: 312.388

Accurate Mass: 309.879564

Percentage Composition: C 30.76%; H 1.61%; Br 51.16%; Cl 11.35%; O 5.12%

Physical Description: Needles (Et₂O)

Melting Point: Mp 80°

>>Derivative: Amide

Molecular Formula: C₈H₇Br₂NO

Molecular Weight: 292.957

Accurate Mass: 290.929436

Percentage Composition: C 32.80%; H 2.41%; Br 54.55%; N 4.78%; O 5.46%

Physical Description: Needles (Et₂O)

Melting Point: Mp 117°

>>Derivative: Nitrile

Synonym(s): 2,6-Dibromo-4-cyanotoluene. 1,3-Dibromo-5-cyano-2-methylbenzene

Molecular Formula: C₈H₅Br₂N

Molecular Weight: 274.942

Accurate Mass: 272.918871

Percentage Composition: C 34.95%; H 1.83%; Br 58.12%; N 5.09%

Physical Description: Needles (EtOH)

Melting Point: Mp 49°

Other Data: Steam-volatile

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1260C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1370A, (*ir*)

Claus, A. *et al.*, *Annalen*, 1891, **265**, 378, (*synth*)

Pearson, D., *J.O.C.*, 1963, **28**, 3147, (*deriv*)