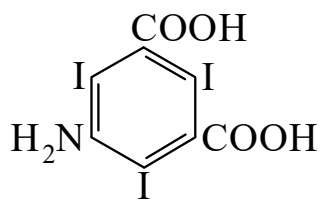




>>Entry Name: 5-Amino-2,4,6-triiodo-1,3-benzenedicarboxylic acid, 9CI



CAS Registry Number: 35453-19-1

Molecular Formula: C₈H₄I₃NO₄

Molecular Weight: 558.837

Accurate Mass: 558.727453

Percentage Composition: C 17.19%; H 0.72%; I 68.13%; N 2.51%; O 11.45%

Physical Description: Cryst. (MeOH aq.)

Aldrich: 44436-7

>>Derivative: Di-Me ester

CAS Registry Number: 154921-11-6

Molecular Formula: C₁₀H₈I₃NO₄

Molecular Weight: 586.891

Accurate Mass: 586.758753

Percentage Composition: C 20.47%; H 1.37%; I 64.87%; N 2.39%; O 10.90%

Physical Description: Plates (MeOH/Et₂O)

Melting Point: Mp 163-164°

>>Derivative: Dichloride

CAS Registry Number: 37441-29-5

Molecular Formula: C₈H₂Cl₂I₃NO₂

Molecular Weight: 595.728

Accurate Mass: 594.659677

Percentage Composition: C 16.13%; H 0.34%; Cl 11.90%; I 63.91%; N 2.35%; O 5.37%

Physical Description: Yellow cryst. solid

Melting Point: Mp 230-231°

References:

Pillai, K.M.R. *et al.*, *J.O.C.*, 1994, **59**, 1344, (*synth, uv, ir, cmr, derivs*)