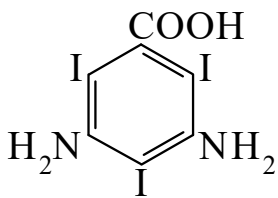




>>Entry Name: 3,5-Diamino-2,4,6-triiodobenzoic acid, 9Cl, 8Cl



CAS Registry Number: 5505-16-8

Related CAS Registry Numbers(s): 8064-12-8 14855-77-7 33954-26-6 50978-11-5

Molecular Formula: C₇H₅I₃N₂O₂

Molecular Weight: 529.842

Accurate Mass: 529.748522

Percentage Composition: C 15.87%; H 0.95%; I 71.85%; N 5.29%; O 6.04%

>>Derivative: *N,N'*-Di-Ac

Synonym(s): Diatrizoic acid, BAN, USAN. Amidotrizoic acid. NSC 262168

CAS Registry Number: 117-96-4

Molecular Formula: C₁₁H₉I₃N₂O₄

Molecular Weight: 613.917

Accurate Mass: 613.769652

Percentage Composition: C 21.52%; H 1.48%; I 62.01%; N 4.56%; O 10.42%

Use/Importance: Radiopaque substance for contrast radiology

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 300°

Calculated Log P Data: Log P -1.81 (calc)

Hazard & Toxicity: Low acute mammalian toxicity (parenterally administered). Adverse renal and other effects reported

Sigma: D9268

>>Derivative: *N,N'*-Di-Ac, Na salt

Synonym(s): Diatrizoate sodium, USAN. Sodium amidotrizoate, INN. Hypaque sodium. Angiografin. Urovist. Cardiografin. Odiston. Renovist. Thixoron. NSC 61815.

Many other names

CAS Registry Number: 737-31-5

Physical Description: Rhombic needles

Melting Point: Mp 261-262 dec.°

Other Data: Light-sensitive. ¹²⁵I and ¹³¹I labelled cpds. are used as radioactive agents

Fluka: 33469

Rare Chemicals Library: S50171-9

Sigma: S4506

>>Derivative: *N,N'*-Di-Ac, meglumine salt (1:1)

Synonym(s): Meglumine diatrizoate

CAS Registry Number: 131-49-7

Physical Description: Rhombic needles

Melting Point: Mp 189-193 dec.°

Other Data: Component of Angiovist 292, Gastrovist, Renovist and Sinografin

Sigma: M5266

>>Derivative: *N,N'*-Dipropanoyl

Synonym(s): Dipotrizoic acid, INN

CAS Registry Number: 85-16-5

Molecular Formula: C₁₃H₁₃I₃N₂O₄

Molecular Weight: 641.97

Accurate Mass: 641.800952

Percentage Composition: C 24.32%; H 2.04%; I 59.30%; N 4.36%; O 9.97%

Use/Importance: Diagnostic aid, radiopaque medium

Physical Description: Brown solid

Melting Point: Mp 340°