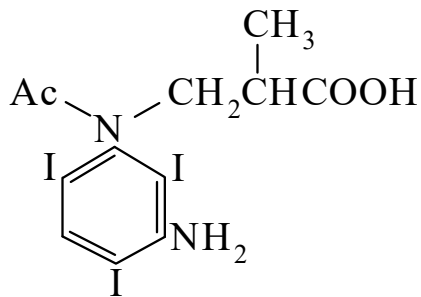




>>Entry Name: Iocetamic acid, BAN, INN, JAN, USAN

Synonym(s): 3-[Acetyl(3-amino-2,4,6-triodophenyl)amino]-2-methylpropanoic acid, 9CI. *N*-Acetyl-*N*-(3-amino-2,4,6-triodophenyl)-2-methyl-β-alanine, 8CI. Cholebrine. Cholimil. Colebrine. DRC 1201. MP 620. TD 73



CAS Registry Number: 16034-77-8

Molecular Formula: C₁₂H₁₃I₃N₂O₃

Molecular Weight: 613.96

Accurate Mass: 613.806037

Percentage Composition: C 23.48%; H 2.13%; I 62.01%; N 4.56%; O 7.82%

Calculated Log P Data: Log P 3.91 (calc)

Hazard & Toxicity: LD₅₀ (rat,orl) 7100 mg/kg

>>Variant: (±)-form

Molecular Formula: C₁₂H₁₃I₃N₂O₃

Molecular Weight: 613.96

Accurate Mass: 613.806037

Percentage Composition: C 23.48%; H 2.13%; I 62.01%; N 4.56%; O 7.82%

Use/Importance: Radiopaque medium

Physical Description: Light cream-coloured powder

Melting Point: Mp 224-225°

Solubility: Sol. Et₂O, EtOH, C₆H₆, insol. H₂O

References:

Korver, J.A., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1968, **87**, 308, (*synth*)

Janbroers, J.M. *et al.*, *Toxicol. Appl. Pharmacol.*, 1969, **14**, 232, (*pharmacol*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 706