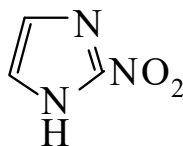




>>Entry Name: 2-Nitroimidazole, 9CI

Synonym(s): Azomycin. Amicin



CAS Registry Number: 527-73-1

Related CAS Registry Numbers(s): 36877-68-6

Molecular Formula: C₃H₃N₃O₂

Molecular Weight: 113.076

Accurate Mass: 113.022527

Percentage Composition: C 31.87%; H 2.67%; N 37.16%; O 28.30%

Biological Source: Produced by *Nocardia* spp., *Streptomyces eurocidicus* and *Pseudomonas fluorescens*

Use/Importance: Antibiotic active against gram-positive organisms

Physical Description: Pale-yellow cryst. (EtOH)

Melting Point: Mp 282 dec.°. Mp 287-288°

Solubility: BERDY SOL: Sol. MeOH, EtOAc, bases; fairly sol. CHCl₃, Et₂O; poorly sol. H₂O, CHCl₃, Me₂CO, hexane, Et₂O

pKa Value: pK_{a1} -0.81; pK_{a2} 7.15 (50% MeOH)

Calculated Log P Data: Log P -0.09 (calc)

UV: [acid] λ_{max} (no shifts reported) (Derep) [base] λ_{max} 223 (ε 3500); 365 (ε 10700) (EtOH/NaOH) (Derep) [neutral] λ_{max} 219 (ε 3900); 315 (ε 8600) (95% EtOH) (Derep) [neutral] λ_{max} 219 (ε 3900); 315 (E1%/1cm 557) (MeOH) (Berdy) [neutral] λ_{max} 314 (E1%/1cm 905) (EtOH) (Berdy) [base] λ_{max} 223 (ε 3500); 365 (ε 10700) (EtOH-NaOH) (Berdy) [base] λ_{max} 362 (E1%/1cm 832) (MeOH-NAOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, orl) 316 mg/kg. Mutagenic props. ; BERDY HAZD : LD₅₀ (mus, ivn) 80 mg/kg

Aldrich: 19565-0

Fluka: 73390

Sigma: N3882

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 618B, (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 489D, (*nmr*)
Nakamura, S. *et al.*, *J. Antibiot., Ser. A*, 1955, **8**, 66, (*isol*)
Beaman, A.G. *et al.*, *J.A.C.S.*, 1965, **87**, 389, (*synth*)
Nakane, A. *et al.*, *J. Biol. Chem.*, 1977, **252**, 5267, (*biosynth*)
Agrawal, K.C. *et al.*, *J. Med. Chem.*, 1979, **22**, 583, (*synth*)
Luijten, W.C. *et al.*, *Org. Mass Spectrom.*, 1982, **17**, 299, (*ms*)
Nair, M.D. *et al.*, *Prog. Drug Res.*, 1983, **27**, 163, (*rev, pharmacol*)
Larsen, I.K., *Acta Cryst. C*, 1984, **40**, 285, (*cryst struct*)
Shoji, T. *et al.*, *J. Antibiot.*, 1989, **42**, 1513, (*isol*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, NHG000