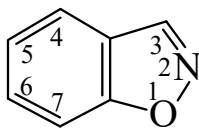




>>Entry Name: 1,2-Benzisoxazole, 9Cl

Synonym(s): Indoxazene. 1-Oxa-2-azaindene



CAS Registry Number: 271-95-4

Molecular Formula: C₇H₅NO

Molecular Weight: 119.123

Accurate Mass: 119.037114

Percentage Composition: C 70.58%; H 4.23%; N 11.76%; O 13.43%

Physical Description: Liq.

Boiling Point: Bp₁₁ 86-87°. Bp₂ 35-38°

Aldrich: 23230-0

Fluka: 12255

>>Derivative: N-Et

Synonym(s): 2-Ethyl-1,2-benzisoxazolium(1+)

CAS Registry Number: 4611-62-5

Molecular Formula: C₉H₁₀NO⁽⁺⁾

Molecular Weight: 148.184

Accurate Mass: 148.076239

Percentage Composition: C 72.95%; H 6.80%; N 9.45%; O 10.80%

Melting Point: Mp 108-110° (as tetrafluoroborate)

Other Data: CAS no. refers to tetrafluoroborate

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 696C, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 195A, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1509B, (*ir*)
Kemp, D.S. *et al.*, *Tetrahedron*, 1965, **21**, 3019, (*synth, uv*)
Wünsch, K.H. *et al.*, *Adv. Heterocycl. Chem.*, 1967, **8**, 277, (*rev*)
Smalley, R.K., *Adv. Heterocycl. Chem.*, 1981, **29**, 1, (*rev*)
Poissonnet, G., *Synth. Commun.*, 1997, **27**, 3839-3846, (*synth, pmr*)