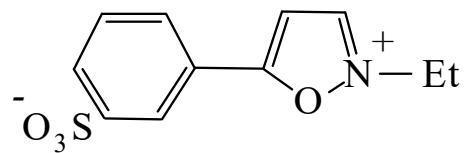




>>Entry Name: **N-Ethyl-5-phenylisoxazolium 3'-sulfonate**

Synonym(s): 2-Ethyl-5-(3-sulfophenyl)isoxazolium inner salt. Woodward's Reagent K. NEPIS



CAS Registry Number: 4156-16-5

Molecular Formula: C₁₁H₁₁NO₄S

Molecular Weight: 253.278

Accurate Mass: 253.040879

Percentage Composition: C 52.16%; H 4.38%; N 5.53%; O 25.27%; S 12.66%

Use/Importance: Peptide condensing agent. Also a reagent for carboxyl group modification in enzymes

Melting Point: Mp 206-208 dec.°

Other Data: Stable, nonhygroscopic

Aldrich: E4526-0

Fluka: 95440

Sigma: E4501

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 637B, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 100C, (*nmr*)

Woodward, R.B. *et al.*, *Tetrahedron, Suppl.*, No. 8, 1966, 321-346, (*synth, rev*)

Woodman, D.J., *Chem. and Biochem. Amino Acids, Pept., Proteins*, (Ed. Weinstein, B.), M. Dekker, 1974, **2**, 207-296, (*rev*)

Brake, A.J. *et al.*, *J. Biol. Chem.*, 1974, **249**, 5452-5457, (*use*)

Org. Synth., 1977, **56**, 88, (*use*)

Arana, J.C. *et al.*, *FEBS Lett.*, 1980, **113**, 319-322, (*use*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 226, (*use*)

Llamas, K. *et al.*, *J.A.C.S.*, 1986, **108**, 5543-5548, (*use*)

Org. Synth., Coll. Vol., 6, 1988, 263-268