



>>Derivative: N-(2-Hydroxyethyl), betaine

Synonym(s): 3-Carboxy-1-(2-hydroxyethyl)pyridinium betaine. **Pyridinebetaine A**

Molecular Formula: C₈H₉NO₃

Molecular Weight: 167.164

Accurate Mass: 167.058244

Percentage Composition: C 57.48%; H 5.43%; N 8.38%; O 28.71%

Biological Source: Isol. from the sponge *Agelas dispar*

Physical Description: Amorph. solid

UV: [neutral] λ_{max} 220 (ε 3000); 266 (ε 2500) (MeOH)

>>Derivative: Butyl ester

CAS Registry Number: 6938-06-3

Molecular Formula: C₁₀H₁₃NO₂

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Melting Point: Mp 252°

Density: d₂₀²⁰ 1.06

Refractive Index: n_D²⁰ 1.4959

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **2**, 785B; 793D; 794A; 797C; 800C; 916C, (*ir*)
- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **3**, 317B; 330B; 331A; 331B; 332B; 336C; 340B; 347C, (*nmr*)
- Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 1546A; 1546C; 1547A; 1549D, (*ir*)
- Org. Synth.*, Coll. Vol., 1, 1932, 385, (*synth*)
- Taylor, E.C. *et al.*, *J.O.C.*, 1954, **19**, 1633, (*oxide*)
- Green, R.W. *et al.*, *J.A.C.S.*, 1956, **78**, 4896, (*deriv*, *uv*, *tautom*)
- Oliveto, E.P., *Chem. Heterocycl. Compd.*, (Part 3), 1962, **14**, 179, (*bibl*)
- Org. Synth.*, Coll. Vol., 4, 1963, 706, (*nitrile*)
- Bild, N. *et al.*, *Helv. Chim. Acta*, 1967, **50**, 1885, (*ms*)
- Poluektov, N.S. *et al.*, *Zh. Anal. Khim.*, 1971, **26**, 541, (*detn*, *U*)
- Pollak, P.I. *et al.*, *Chem. Heterocycl. Compd.*, Suppl. 3, 1974, **14**, (*bibl*)
- Paraskewas, S., *Synthesis*, 1974, 819, (*synth*)
- Kirk-Othmer Encycl. Chem. Technol.*, 3rd edn., Wiley, 1978, **24**, 59, (*rev*)
- Belg. Pat.*, 1980, 618 968; *CA*, **58**, 12375e, (*oxide*)
- Dommissie, R. *et al.*, *Heterocycles*, 1981, **16**, 1893, (*cmr*)
- Staedeli, W. *et al.*, *Org. Magn. Reson.*, 1981, **15**, 106, (*N-15 nmr*)
- Kutoglu, A. *et al.*, *Acta Cryst. C*, 1983, **39**, 232, (*cryst struct*)
- Hotz, W., *Adv. Lipid Res.*, 1983, **20**, 195, (*rev*, *pharmacol*)
- Weiner, M. *et al.*, *Clin. Pharmacol. Vol. 1: Nicotinic Acid Nutrient-Cofactor-Drug*, Dekker, N.Y., 1983, (*book*)
- Sauberlich, H.E. *et al.*, *Coenzymes Cofactors*, 1987, **2**, 599; 627, (*revs*)
- Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, 1987, 394, (*synonyms*)
- El-Shahawy, A.S. *et al.*, *Spectrochim. Acta A*, 1987, **43**, 1371, (*uv*)
- Cossio, F.P. *et al.*, *Tetrahedron*, 1987, **43**, 3963, (*synth*)
- Maumy, M. *et al.*, *Synthesis*, 1989, 451, (*nitrile*)
- de Oliveira, S.M. *et al.*, *Org. Mass Spectrom.*, 1991, **26**, 855, (*ms*)
- Martindale, The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, 1993, 1045
- Chattopadhyay, S. *et al.*, *Spectrochim. Acta A*, 1993, **49**, 589, (*ir*, *Raman*)
- Encyclopedia of Food and Color Additives*, (ed. Burdock, G.A.), CRC Press, 1997, 1806-1807; 1951-1973, (*props*, *use*, *Me ester*)
- Ohshima, N. *et al.*, *Phytochemistry*, 1997, **44**, 1483, (*glucosyl ester*)
- Cafieri, F. *et al.*, *J. Nat. Prod.*, 1998, **61**, 1171-1173, (*Pyridinebetaine A*)
- Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, NCQ900; NDV000; NDU500; NDW500