



10 buffer) (Berdy)

>>Derivative: 4-Me ether, *N,N,N*-tri-Me, betaine

CAS Registry Number: 153343-23-8

Extra CAS Registry Numbers(s): 165329-90-8

Molecular Formula: C₁₃H₁₈BrNO₃

Molecular Weight: 316.194

Accurate Mass: 315.067005

Percentage Composition: C 49.38%; H 5.74%; Br 25.27%; N 4.43%; O 15.18%

Biological Source: Isol. from *Pseudoceratina crassa*

Optical Rotation: [α]_D -9 (MeOH)

Solubility: BERDY SOL: Sol. H₂O, MeOH

UV: [neutral] $\lambda_{\max}$ 277 (ϵ 1260) (H₂O) [neutral] $\lambda_{\max}$ 277 (ϵ 1260) (H₂O) (Berdy)

>>Variant: ($\pm$)-form

CAS Registry Number: 54788-30-6

Molecular Formula: C₉H₁₀BrNO₃

Molecular Weight: 260.087

Accurate Mass: 259.004405

Percentage Composition: C 41.56%; H 3.88%; Br 30.72%; N 5.39%; O 18.45%

Melting Point: Mp 245-246°

References:

- Johnson, T.B. *et al.*, *J.A.C.S.*, 1912, **34**, 1061, (*synth*)
Welinder, B.S., *Biochim. Biophys. Acta*, 1972, **279**, 491, (*isol, ms, synth*)
Firnau, G. *et al.*, *Bioinorg. Chem.*, 1973, **2**, 167; *CA*, **79**, 124178q
McCord, T.J. *et al.*, *J. Med. Chem.*, 1975, **18**, 26, (*synth*)
Albrizio, S. *et al.*, *Tetrahedron*, 1994, **50**, 783-788, (*isol, betaines*)
Gao, H. *et al.*, *Tetrahedron*, 1999, **55**, 9717-9726, (*abs config*)