



>>Entry Name: 1,3,5-Triethynylbenzene, 9CI

CAS Registry Number: 7567-63-7

Molecular Formula: C₁₂H₆

Molecular Weight: 150.179

Accurate Mass: 150.04695

Percentage Composition: C 95.97%; H 4.03%

Physical Description: Needles (EtOH), bright yellow cryst. (hexane)

Melting Point: Mp 105-107° (94-96°)

Hazard & Toxicity: An explosion hazard has been reported but this appears to be erroneous

References:

Hubel, W. *et al.*, *Chem. Ber.*, 1963, **96**, 930

Effenberger, F. *et al.*, *Chem. Ber.*, 1973, **106**, 511

Weber, E. *et al.*, *J.C.S. Perkin 2*, 1988, 1251, (*synth*)

Royles, B.J.L. *et al.*, *J.C.S. Perkin 1*, 1994, 355, (*synth*)

Andersen, H.L. *et al.*, *J.C.S. Perkin 1*, 1995, 2275, (*synth*, *ir*, *pmr*)

MacBride, J.A.H. *et al.*, *Synth. Commun.*, 1996, **26**, 2309, (*synth*)

Weiss, H.-C. *et al.*, *Chem. Comm.*, 1997, 1703-1704, (*cryst struct*)

Mongin, O. *et al.*, *J.O.C.*, 1998, **63**, 5568-5580, (*synth*)