



>>Entry Name: 5-Methylbenzotriazole, 9CI

CAS Registry Number: 136-85-6

Related CAS Registry Numbers(s): 64665-57-2

Extra CAS Registry Numbers(s): 29385-43-1

Molecular Formula: $C_7H_7N_3$

Molecular Weight: 133.152

Accurate Mass: 133.063997

Percentage Composition: C 63.14%; H 5.30%; N 31.56%

Melting Point: Mp 83-84°

Other Data: An oil assigned this struct. was shown to be 1-Azido-4-methylbenzene [BHX78-T](#)

Hazard & Toxicity: LD₅₀ (rat, orl) 1600 mg/kg

Aldrich: 19630-4

Rare Chemicals Library: S56653-5

>>Variant: 1*H*-form

Molecular Formula: $C_7H_7N_3$

Molecular Weight: 133.152

Accurate Mass: 133.063997

Percentage Composition: C 63.14%; H 5.30%; N 31.56%

>>Derivative: 1-Amino

CAS Registry Number: 21991-63-9

Molecular Formula: $C_7H_8N_4$

Molecular Weight: 148.167

Accurate Mass: 148.074896

Percentage Composition: C 56.74%; H 5.44%; N 37.81%

Physical Description: Needles (C_6H_6 /petrol)

Melting Point: Mp 87-88°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 188C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 694C, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1508C, (*ir*)

Morgan, G.T. *et al.*, *J.C.S.*, 1913, **103**, 1391

Campbell, C.D. *et al.*, *J.C.S.(C)*, 1969, 742

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, MHK250