>>**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: LD_{50} (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)*
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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