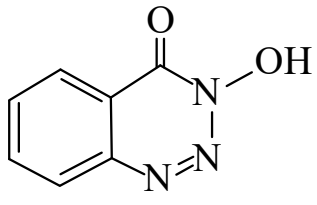
>>**Entry Name: 3-Hydroxy-1,2,3-benzotriazin-4(3*H*)-one,** 9CI



CAS Registry Number: 28230-32-2

Molecular Formula: $C_7H_5N_3O_2$
Molecular Weight: 163.135
Accurate Mass: 163.038177
Percentage Composition: C 51.54%; H 3.09%; N 25.76%; O 19.61%

Use/Importance: Reagent for peptide synth.
Physical Description: Needles (EtOH)
Melting Point: Mp 182-182.5 dec.°

Aldrich: 32796-4
Fluka: 37305
Sigma: H6770

>>**Derivative:** *O*-Ac
Synonym(s): 3-Acetoxy-1,2,3-benzotriazin-4(3*H*)-one

Molecular Formula: $C_9H_7N_3O_3$
Molecular Weight: 205.173
Accurate Mass: 205.048742
Percentage Composition: C 52.69%; H 3.44%; N 20.48%; O 23.39%
Physical Description: Prisms (C_6H_6)
Melting Point: Mp 174-175°

>>**Derivative:** Me ether
Synonym(s): 3-Methoxy-1,2,3-benzotriazin-4(3*H*)-one

Molecular Formula: $C_8H_7N_3O_2$
Molecular Weight: 177.162
Accurate Mass: 177.053827
Percentage Composition: C 54.24%; H 3.98%; N 23.72%; O 18.06%
Physical Description: Needles (EtOH)
Melting Point: Mp 134-135°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 480A, *(nmr)*
König, W. *et al.*, *Chem. Ber.*, 1970, **103**, 2034-2040, *(use)*
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 342, *(synth, use)*
Ahern, T.P. *et al.*, *Can. J. Chem.*, 1977, **55**, 630-639, *(synth, O-Ac, Me ether)*
Hunt, W.E. *et al.*, *Acta Cryst. C*, 1983, **39**, 738-740, *(cryst struct)*
Jakobsen, M.H. *et al.*, *Synthesis*, 1990, 1008-1010, *(synth, ir, uv, pmr, cmr)*