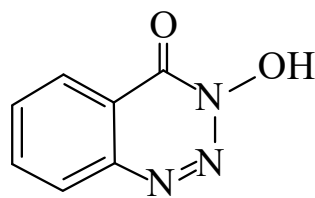




>>Entry Name: 3-Hydroxy-1,2,3-benzotriazin-4(3H)-one, 9Cl



CAS Registry Number: 28230-32-2

Molecular Formula: C<sub>7</sub>H<sub>5</sub>N<sub>3</sub>O<sub>2</sub>

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(3H)-one

Molecular Formula: C<sub>9</sub>H<sub>7</sub>N<sub>3</sub>O<sub>3</sub>

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<sub>6</sub>H<sub>6</sub>)

Melting Point: Mp 174-175°

>>Derivative: Me ether

Synonym(s): 3-Methoxy-1,2,3-benzotriazin-4(3H)-one

Molecular Formula: C<sub>8</sub>H<sub>7</sub>N<sub>3</sub>O<sub>2</sub>

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)