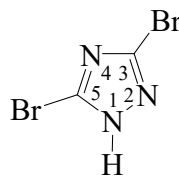




>>Entry Name: 3,5-Dibromo-1*H*-1,2,4-triazole



CAS Registry Number: 7411-23-6

Molecular Formula: C<sub>2</sub>HBr<sub>2</sub>N<sub>3</sub>

Molecular Weight: 226.858

Accurate Mass: 224.893719

Percentage Composition: C 10.59%; H 0.44%; Br 70.44%; N 18.52%

Physical Description: Needles

Melting Point: Mp 211-212° (EtOH aq. or CHCl<sub>3</sub>)

Rare Chemicals Library: S93456-9

>>Derivative: *N*<sup>1</sup>-Me

Synonym(s): 3,5-Dibromo-1-methyl-1*H*-1,2,4-triazole

CAS Registry Number: 23579-79-5

Molecular Formula: C<sub>3</sub>H<sub>3</sub>Br<sub>2</sub>N<sub>3</sub>

Molecular Weight: 240.885

Accurate Mass: 238.909369

Percentage Composition: C 14.96%; H 1.26%; Br 66.34%; N 17.44%

Physical Description: Cryst. (hexane)

Melting Point: Mp 64-65°

>>Variant: 4*H*-form

Molecular Formula: C<sub>2</sub>HBr<sub>2</sub>N<sub>3</sub>

Molecular Weight: 226.858

Accurate Mass: 224.893719

Percentage Composition: C 10.59%; H 0.44%; Br 70.44%; N 18.52%

>>Derivative: *N*<sup>4</sup>-Me

Synonym(s): 3,5-Dibromo-4-methyl-4*H*-1,2,4-triazole

CAS Registry Number: 56616-88-7

Molecular Formula: C<sub>3</sub>H<sub>3</sub>Br<sub>2</sub>N<sub>3</sub>

Molecular Weight: 240.885

Accurate Mass: 238.909369

Percentage Composition: C 14.96%; H 1.26%; Br 66.34%; N 17.44%

Physical Description: Cryst. (CHCl<sub>3</sub>)

Melting Point: Mp 166°

#### References:

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Browne, E.J. *et al.*, *J.C.S.(C)*, 1969, 1056-1060, (*ir*)

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