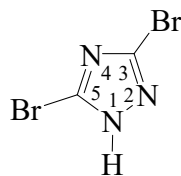




>>Entry Name: 3,5-Dibromo-1*H*-1,2,4-triazole



CAS Registry Number: 7411-23-6

Molecular Formula: C₂HBr₂N₃

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 CHCl₃)

Rare Chemicals Library: S93456-9

>>Derivative: *N*¹-Me

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

CAS Registry Number: 23579-79-5

Molecular Formula: C₃H₃Br₂N₃

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: C₂HBr₂N₃

Molecular Weight: 226.858

Accurate Mass: 224.893719

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

>>Derivative: *N*⁴-Me

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

CAS Registry Number: 56616-88-7

Molecular Formula: C₃H₃Br₂N₃

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. (CHCl₃)

Melting Point: Mp 166°

References:

Kröger, C.-F. *et al.*, *Z. Chem.*, 1965, **5**, 381-382, (*pKa*)

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

Miethchen, R. *et al.*, *Z. Chem.*, 1969, **9**, 300-302, (*1-Me*)

Bernardini, A. *et al.*, *Bull. Soc. Chim. Fr.*, 1975, 647-653, (*4-Me*)

Volkonen, J. *et al.*, *Acta Chem. Scand., Ser. A*, 1985, **39**, 711-716, (*synth, props, ir*)