



>>Entry Name: 2-Amino-5-bromopyrimidine, 8Cl

Synonym(s): 5-Bromo-2-pyrimidinamine, 9Cl

CAS Registry Number: 7752-82-1

Molecular Formula: C<sub>4</sub>H<sub>4</sub>BrN<sub>3</sub>

Molecular Weight: 174

Accurate Mass: 172.978858

Percentage Composition: C 27.61%; H 2.32%; Br 45.92%; N 24.15%

Physical Description: Lustrous plates (EtOH aq.)

Melting Point: Mp 242-244°

Other Data: Sublimes

Aldrich: 30352-6

>>Derivative: Hydrochloride

CAS Registry Number: 99651-86-2

Melting Point: Mp 190 dec.°

>>Derivative: *N*-(4-Methylbenzenesulfonyl)

Molecular Formula: C<sub>11</sub>H<sub>10</sub>BrN<sub>3</sub>O<sub>2</sub>S

Molecular Weight: 328.189

Accurate Mass: 326.987708

Percentage Composition: C 40.26%; H 3.07%; Br 24.35%; N 12.80%; O 9.75%; S 9.77%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 254-256°

>>Derivative: *N,N*-Di-Me

CAS Registry Number: 38696-21-8

Molecular Formula: C<sub>6</sub>H<sub>8</sub>BrN<sub>3</sub>

Molecular Weight: 202.053

Accurate Mass: 201.010158

Percentage Composition: C 35.67%; H 3.99%; Br 39.55%; N 20.80%

Physical Description: Needles

Melting Point: Mp 79.5-80.5°

#### References:

- Nishiwaki, T., *Tetrahedron*, 1966, **22**, 2401, (*uv*)  
Khmelnitskii, R.A. *et al.*, *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1973, 1528, (*ms*)  
Jovanovic, M.V., *Heterocycles*, 1983, **20**, 2011, (*synth*)  
Paudler, W.W. *et al.*, *J.O.C.*, 1983, **48**, 1064, (*synth, pmr*)  
Fichter, R. *et al.*, *J. Chem. Educ.*, 1985, **62**, 905, (*synth*)  
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Kanie, K. *et al.*, *Bull. Chem. Soc. Jpn.*, 1999, **72**, 2523-2535, (*N,N-di-Me*)  
Acero-Alarcon, A. *et al.*, *Synthesis*, 1999, 2124-2130, (*N-tosyl*)