



**>>Entry Name: 1-Amino-4-bromoanthraquinone**

**Synonym(s):** 1-Amino-4-bromo-9,10-anthracenedione, 9Cl

**CAS Registry Number:** 81-62-9

**Related CAS Registry Numbers(s):** 126871-79-2

**Molecular Formula:** C<sub>14</sub>H<sub>8</sub>BrNO<sub>2</sub>

**Molecular Weight:** 302.127

**Accurate Mass:** 300.99384

**Percentage Composition:** C 55.66%; H 2.67%; Br 26.45%; N 4.64%; O 10.59%

**Use/Importance:** Dye intermed.

**Physical Description:** Cryst. (AcOH)

**Melting Point:** Mp 178.5-179.5° (172-175°)

**pKa Value:** pK<sub>a</sub> -1.12

**Rare Chemicals Library:** S92275-7

**>>Derivative: N-Ac**

**Molecular Formula:** C<sub>16</sub>H<sub>10</sub>BrNO<sub>3</sub>

**Molecular Weight:** 344.164

**Accurate Mass:** 343.004405

**Percentage Composition:** C 55.84%; H 2.93%; Br 23.22%; N 4.07%; O 13.95%

**Melting Point:** Mp 222-224°

**>>Derivative: N-Benzoyl**

**Molecular Formula:** C<sub>21</sub>H<sub>12</sub>BrNO<sub>3</sub>

**Molecular Weight:** 406.235

**Accurate Mass:** 405.020055

**Percentage Composition:** C 62.09%; H 2.98%; Br 19.67%; N 3.45%; O 11.82%

**Physical Description:** Yellow needles

**Melting Point:** Mp 230-231° (225-227°)

**>>Derivative: N-Me**

**CAS Registry Number:** 128-93-8

**Molecular Formula:** C<sub>15</sub>H<sub>10</sub>BrNO<sub>2</sub>

**Molecular Weight:** 316.153

**Accurate Mass:** 315.00949

**Percentage Composition:** C 56.99%; H 3.19%; Br 25.27%; N 4.43%; O 10.12%

**Physical Description:** Red-brown needles (Py)

**Melting Point:** Mp 195-196°

**Hazard & Toxicity:** Mild eye irritant

**Rare Chemicals Library:** S26364-8

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

**Molecular Formula:** C<sub>16</sub>H<sub>12</sub>BrNO<sub>2</sub>

**Molecular Weight:** 330.18

**Accurate Mass:** 329.02514

**Percentage Composition:** C 58.20%; H 3.66%; Br 24.20%; N 4.24%; O 9.69%

**Melting Point:** Mp 178°

**References:**

Gasparic, J. *et al.*, *Coll. Czech. Chem. Comm.*, 1962, **27**, 46, (*synth*)

Arai, S. *et al.*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 547, (*synth, uv*)

Gornostaev, L.M. *et al.*, *Zh. Org. Khim.*, 1980, **16**, 642, (*synth*)

Bethell, D. *et al.*, *J.C.S. Perkin 2*, 1985, 1789, (*bibl*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BNN550