



>>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: C₁₄H₈BrNO₂

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_a -1.12

Rare Chemicals Library: S92275-7

>>Derivative: *N*-Ac

Molecular Formula: C₁₆H₁₀BrNO₃

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: C₂₁H₁₂BrNO₃

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: C₁₅H₁₀BrNO₂

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: C₁₆H₁₂BrNO₂

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