



>>Entry Name: 2-Amino-4-hydroxybenzoic acid

Synonym(s): 4-Hydroxyanthranilic acid

CAS Registry Number: 38160-63-3

Molecular Formula: C₇H₇NO₃

Molecular Weight: 153.137

Accurate Mass: 153.042594

Percentage Composition: C 54.90%; H 4.61%; N 9.15%; O 31.34%

Physical Description: Needles (H₂O)

Melting Point: Mp 148° (dec.)

>>Derivative: Hydrochloride

Physical Description: Needles

>>Derivative: Me ester

Molecular Formula: C₈H₉NO₃

Molecular Weight: 167.164

Accurate Mass: 167.058244

Percentage Composition: C 57.48%; H 5.43%; N 8.38%; O 28.71%

Physical Description: Needles

Melting Point: Mp 132-133°

>>Derivative: Me ether

Synonym(s): 2-Amino-4-methoxybenzoic acid. 2-Aminoanisic acid. 4-Methoxyanthranilic acid

CAS Registry Number: 4294-95-5

Molecular Formula: C₈H₉NO₃

Molecular Weight: 167.164

Accurate Mass: 167.058244

Percentage Composition: C 57.48%; H 5.43%; N 8.38%; O 28.71%

Physical Description: Plates (EtOH)

Melting Point: Mp 166° (dec.). Mp 190°

pKa Value: pK_{a1} 2.06; pK_{a2} 4.88 (25°, 0.1M KCl)

>>Derivative: *N*-(4-Hydroxycinnamoyl) (*E*-)

Synonym(s): 4-Hydroxy-*N*-(4-hydroxycinnamoyl)anthranilic acid. **Avenanthramide G**

Molecular Formula: C₁₆H₁₃NO₅

Molecular Weight: 299.282

Accurate Mass: 299.079374

Percentage Composition: C 64.21%; H 4.38%; N 4.68%; O 26.73%

Biological Source: Stress metab. in oats (*Avena sativa*) induced by Victorin M [JTT63-H](#)

Physical Description: Cryst. + &lqu; MeOH (MeOH/1% AcOH aq.)

Melting Point: Mp 290-291°

References:

CRC Atlas of Spectral Data and Physical Constants, b843, (uv)

Drain, D.G. *et al.*, *J.C.S.*, 1949, 1489, (synth)

van der Stelt, C. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1953, **72**, 195, (synth)

Jilek, J. *et al.*, *Coll. Czech. Chem. Comm.*, 1985, **50**, 519, (synth, uv, ir, pmr, deriv)

Paulidis, V.H. *et al.*, *Synth. Commun.*, 1994, **24**, 533, (Me ether, synth, ir, pmr, cmr)

Miyagawa, H. *et al.*, *Phytochemistry*, 1996, **41**, 1473, (Avenanthramide G)

Boojamra, C.G. *et al.*, *J.O.C.*, 1997, **62**, 1240-1256, (Me ether)