



>>Entry Name: 4-Hydroxy-3,5-dimethylbenzaldehyde, 9CI

Synonym(s): 3,5-Dimethyl-*p*-hydroxybenzaldehyde, 9CI. 4-Formyl-2-hydroxy-*m*-xylene. *p*-Hydroxymesitylenic aldehyde

CAS Registry Number: 2233-18-3

Molecular Formula: C<sub>9</sub>H<sub>10</sub>O<sub>2</sub>

Molecular Weight: 150.177

Accurate Mass: 150.06808

Percentage Composition: C 71.98%; H 6.71%; O 21.31%

Physical Description: Leaflets (EtOH aq.)

Melting Point: Mp 115-116°

pKa Value: pK<sub>a1</sub> 7.74 (25°)

Aldrich: 14039-2

Fluka: 40700

Rare Chemicals Library: S41443-3

>>Derivative: Oxime

Molecular Formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>

Molecular Weight: 165.191

Accurate Mass: 165.078979

Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%

Physical Description: Needles (C<sub>6</sub>H<sub>6</sub>/Et<sub>2</sub>O)

Melting Point: Mp 169.5°

>>Derivative: Phenylhydrazone

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 143°

>>Derivative: Benzoyl

Molecular Formula: C<sub>16</sub>H<sub>14</sub>O<sub>3</sub>

Molecular Weight: 254.285

Accurate Mass: 254.094295

Percentage Composition: C 75.58%; H 5.55%; O 18.88%

Physical Description: Cryst. (petrol)

Melting Point: Mp 105°

>>Derivative: Me ether

Synonym(s): 4-Methoxy-3,5-dimethylbenzaldehyde. 3,5-Dimethylanisaldehyde

CAS Registry Number: 39250-90-3

Molecular Formula: C<sub>10</sub>H<sub>12</sub>O<sub>2</sub>

Molecular Weight: 164.204

Accurate Mass: 164.08373

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Boiling Point: Bp 257°

#### References:

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 965A, (*nmr*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 1305B, (*ir*)

*Aldrich Library of Infrared Spectra*, 3rd edn., 1981, 922E, (*ir*)

Thiele, J. *et al.*, *Annalen*, 1900, **311**, 367, (*synth*)

Gattermann, L., *Annalen*, 1907, **357**, 363, (*synth*)

Baik, W. *et al.*, *J.O.C.*, 2000, **65**, 108-115, (*synth*, *pmr*)