



>>Entry Name: 2,4,6-Trimethylaniline

Synonym(s): 2,4,6-Trimethylbenzenamine, 9CI. Mesidine. Aminomesitylene. Mesitylamine

CAS Registry Number: 88-05-1

Molecular Formula: C<sub>9</sub>H<sub>13</sub>N

Molecular Weight: 135.208

Accurate Mass: 135.104799

Percentage Composition: C 79.95%; H 9.69%; N 10.36%

Boiling Point: Bp 232-233°

pKa Value: pK<sub>a</sub> 4.38 (25°)

Hazard & Toxicity: Skin and severe eye irritant. LD<sub>50</sub> (rat, orl) 743 mg/kg

Aldrich: 13217-9

Fluka: 92290

Sigma: T4127

>>Derivative: Picrate

Physical Description: Yellow prisms (EtOH/petrol)

Melting Point: Mp 189-191°

>>Derivative: *N*-Ac

Synonym(s): *N*-(2,4,6-Trimethylphenyl)acetamide. Acetomesidide

CAS Registry Number: 5096-21-9

Molecular Formula: C<sub>11</sub>H<sub>15</sub>NO

Molecular Weight: 177.246

Accurate Mass: 177.115364

Percentage Composition: C 74.54%; H 8.53%; N 7.90%; O 9.03%

Physical Description: Prisms (EtOH)

Melting Point: Mp 216-217°

>>Derivative: *N*-Benzoyl

Synonym(s): *N*-(2,4,6-Trimethylphenyl)benzamide, 9CI. Benzomesidide

CAS Registry Number: 4476-12-4

Molecular Formula: C<sub>16</sub>H<sub>17</sub>NO

Molecular Weight: 239.316

Accurate Mass: 239.131014

Percentage Composition: C 80.30%; H 7.16%; N 5.85%; O 6.69%

Physical Description: Needles (EtOH)

Melting Point: Mp 204°

Rare Chemicals Library: S70921-2

>>Derivative: 4-Methylbenzenesulfonyl

Physical Description: Needles (EtOH)

Melting Point: Mp 167°

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

Synonym(s): *N,N*,2,4,6-Pentamethylaniline, 8CI. *N,N*,2,4,6-Pentamethylbenzenamine, 9CI

CAS Registry Number: 13021-15-3

Molecular Formula: C<sub>11</sub>H<sub>17</sub>N

Molecular Weight: 163.262

Accurate Mass: 163.136099

Percentage Composition: C 80.93%; H 10.49%; N 8.58%

Physical Description: Liq.

Boiling Point: Bp 213-215°

Density: d 0.91

Refractive Index: n<sub>D</sub><sup>20</sup> 1.5120

References: