



**CAS Registry Number:** 21245-02-3

**Type of Compound Code(s):** XA6420

**Molecular Formula:** C<sub>17</sub>H<sub>27</sub>NO<sub>2</sub>

**Molecular Weight:** 277.406

**Accurate Mass:** 277.204179

**Percentage Composition:** C 73.61%; H 9.81%; N 5.05%; O 11.54%

**Use/Importance:** Extensively used in sunscreen preparations

**Calculated Log P Data:** Log P 6.19 (calc)

**Hazard & Toxicity:** Contact- and photo-allergic responses reported from topical use. Sunlight-induced mutagenic props. reported

**Aldrich:** 43739-5

>>Derivative: Octyl ester

**Synonym(s):** Octyl 4-(dimethylamino)benzoate

**CAS Registry Number:** 58817-05-3

**Molecular Formula:** C<sub>17</sub>H<sub>27</sub>NO<sub>2</sub>

**Molecular Weight:** 277.406

**Accurate Mass:** 277.204179

**Percentage Composition:** C 73.61%; H 9.81%; N 5.05%; O 11.54%

**Use/Importance:** Sunscreen agent for cosmetics

>>Derivative: Chloride

**CAS Registry Number:** 4755-50-4

**Molecular Formula:** C<sub>9</sub>H<sub>10</sub>ClNO

**Molecular Weight:** 183.637

**Accurate Mass:** 183.045091

**Percentage Composition:** C 58.87%; H 5.49%; Cl 19.31%; N 7.63%; O 8.71%

**Physical Description:** Cryst.

**Melting Point:** Mp 147-149°

>>Derivative: Amide

**CAS Registry Number:** 6083-47-2

**Molecular Formula:** C<sub>9</sub>H<sub>12</sub>N<sub>2</sub>O

**Molecular Weight:** 164.207

**Accurate Mass:** 164.094963

**Percentage Composition:** C 65.83%; H 7.37%; N 17.06%; O 9.74%

**Physical Description:** Cryst. (EtOH aq.)

**Melting Point:** Mp 206°

>>Derivative: Nitrile

**Synonym(s):** 4-Dimethylaminobenzonitrile. 4-Cyanodimethylaniline

**CAS Registry Number:** 1197-19-9

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

**Molecular Weight:** 146.191

**Accurate Mass:** 146.084398

**Percentage Composition:** C 73.94%; H 6.89%; N 19.16%

**Physical Description:** Yellow cryst.

**Melting Point:** Mp 75.6°

**Boiling Point:** Bp 318°

**Aldrich:** D13950-5

**Fluka:** 39140

#### References: