



CAS Registry Number: 21245-02-3
Type of Compound Code(s): XA6420
Molecular Formula: C₁₇H₂₇NO₂
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: C₁₇H₂₇NO₂
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: C₉H₁₀ClNO
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: C₉H₁₂N₂O
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: C₉H₁₀N₂
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: