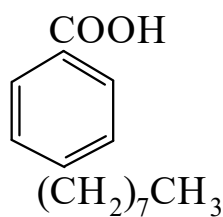




>>Entry Name: 4-Octylbenzoic acid, 9CI



CAS Registry Number: 3575-31-3

Molecular Formula: C₁₅H₂₂O₂

Molecular Weight: 234.338

Accurate Mass: 234.16198

Percentage Composition: C 76.88%; H 9.46%; O 13.66%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 139°. Mp 99-100°

pKa Value: pK_a 6.5 (25°)

Aldrich: 37420-2

Fluka: 75002

>>Derivative: Chloride

CAS Registry Number: 50606-97-8

Molecular Formula: C₁₅H₂₁ClO

Molecular Weight: 252.783

Accurate Mass: 252.128092

Percentage Composition: C 71.27%; H 8.37%; Cl 14.02%; O 6.33%

Boiling Point: Bp₁₂ 188°

>>Derivative: Amide

Molecular Formula: C₁₅H₂₃NO

Molecular Weight: 233.353

Accurate Mass: 233.177964

Percentage Composition: C 77.21%; H 9.93%; N 6.00%; O 6.86%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 139-140°

>>Derivative: Anilide

Molecular Formula: C₂₁H₂₇NO

Molecular Weight: 309.45

Accurate Mass: 309.209264

Percentage Composition: C 81.51%; H 8.79%; N 4.53%; O 5.17%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 102°

References:

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Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, OEQ000