



>>Entry Name: Acetophenone, 8Cl

Synonym(s): 1-Phenylethanone, 9Cl. Methyl phenyl ketone. Hypnone. Acetylbenzene

CAS Registry Number: 98-86-2

Related CAS Registry Numbers(s): 19547-00-3 59130-82-4

PhCOCH₃

Molecular Formula: C₈H₈O

Molecular Weight: 120.151

Accurate Mass: 120.057515

Percentage Composition: C 79.97%; H 6.71%; O 13.32%

Biological Source: Isol. from essential oils. Obt. comly as byprod. in the Hock phenol synthesis

Use/Importance: Has soporific props. Solvent, resin intermed. Photochemical sensitiser. Used in extraction separation of Se from Te. Used in perfumery

Physical Description: Plates (freq. obt. as liq.) with penetrating sweet odour

Melting Point: Mp 20°

Boiling Point: Bp 202°. Bp₅ 67°

Solubility: Sol. EtOH, Et₂O; insol. H₂O

Density: d₄²⁰ 1.029

pKa Value: pK_{a1} -6.4 (25°, H₂SO₄ aq.)

Refractive Index: n_D²⁰ 1.5342

Hazard & Toxicity: Fl. p. 77°, autoignition temp. 570°. Skin and severe eye irritant. LD₅₀ (rat, orl) 815 mg/kg

Aldrich: W20090-5

Fluka: 800

Sigma: A1890

Supelco: R52-5110

>>Derivative: (E)-Oxime

Synonym(s): *syn*-Oxime

CAS Registry Number: 10341-75-0

Extra CAS Registry Numbers(s): 613-91-2

Molecular Formula: C₈H₉NO

Molecular Weight: 135.165

Accurate Mass: 135.068414

Percentage Composition: C 71.09%; H 6.71%; N 10.36%; O 11.84%

Melting Point: Mp 59.5-60.5°

pKa Value: pK_{a1} 11.35