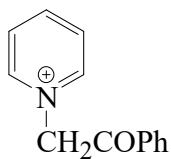




>>Entry Name: 1-(2-Oxo-2-phenylethyl)pyridinium(1+)

Synonym(s): N-Phenacylpyridinium(1+)



CAS Registry Number: 18413-03-1

Molecular Formula: C₁₃H₁₂NO⁽⁺⁾

Molecular Weight: 198.244

Accurate Mass: 198.091889

Percentage Composition: C 78.76%; H 6.10%; N 7.07%; O 8.07%

>>Derivative: Chloride

CAS Registry Number: 20517-71-9

Molecular Formula: C₁₃H₁₂ClNO

Molecular Weight: 233.697

Accurate Mass: 233.060741

Percentage Composition: C 66.81%; H 5.18%; Cl 15.17%; N 5.99%; O 6.85%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 109-110°

>>Derivative: Bromide

CAS Registry Number: 16883-69-5

Molecular Formula: C₁₃H₁₂BrNO

Molecular Weight: 278.148

Accurate Mass: 277.030225

Percentage Composition: C 56.14%; H 4.35%; Br 28.73%; N 5.04%; O 5.75%

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 202-203° (200-202°)

>>Derivative: Iodide

CAS Registry Number: 1137-94-6

Molecular Formula: C₁₃H₁₂INO

Molecular Weight: 325.148

Accurate Mass: 324.996362

Percentage Composition: C 48.02%; H 3.72%; I 39.03%; N 4.31%; O 4.92%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 218-219°

>>Derivative: Perchlorate

CAS Registry Number: 27387-18-4

Molecular Formula: C₁₃H₁₂ClNO₅

Molecular Weight: 297.694

Accurate Mass: 297.040401

Percentage Composition: C 52.45%; H 4.06%; Cl 11.91%; N 4.71%; O 26.87%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 189-190°

References:

Van der Meulen, P.A. *et al.*, *J.A.C.S.*, 1932, **54**, 4407-4409, (*chloride*)

Baker, J.W., *J.C.S.*, 1932, 1148-1157, (*bromide*)

King, L.C., *J.A.C.S.*, 1944, **66**, 894-895, (*iodide, perchlorate*)

Phillips, W.G. *et al.*, *J.O.C.*, 1970, **35**, 3144, (*bromide, synth, pmr*)