



>>Entry Name: 2'-Hydroxy-5'-nitroacetophenone

Synonym(s): 1-(2-Hydroxy-5-nitrophenyl)ethanone, 9CI

CAS Registry Number: 1450-76-6

Molecular Formula: C₈H₇NO₄

Molecular Weight: 181.148

Accurate Mass: 181.037509

Percentage Composition: C 53.04%; H 3.89%; N 7.73%; O 35.33%

Physical Description: Needles (AcOH)

Melting Point: Mp 101-102°. Mp 111-112°

pKa Value: pK_a 7.05 (25°)

Other Data: Steam-volatile

>>Derivative: Oxime

CAS Registry Number: 42524-25-4

Molecular Formula: C₈H₈N₂O₄

Molecular Weight: 196.162

Accurate Mass: 196.048408

Percentage Composition: C 48.98%; H 4.11%; N 14.28%; O 32.62%

Physical Description: Needles (EtOH or C₆H₆)

Melting Point: Mp 231°

References:

Lindemann, H. *et al.*, *J. Prakt. Chem.*, 1929, **122**, 214-231, (*synth, oxime*)

Allen, D. *et al.*, *J.C.S.*, 1949, 821-825, (*synth*)

Joshi, S.S. *et al.*, *J.A.C.S.*, 1954, **76**, 4993-4994, (*synth*)

Chang, C.T. *et al.*, *J.C.S.*, 1961, 3414-3417, (*synth*)

Cushman, M. *et al.*, *J. Med. Chem.*, 1994, **37**, 3353-3362, (*synth, ir, pmr*)

Joshi, R.A. *et al.*, *Org. Process Res. Dev.*, 2001, **5**, 176-178, (*synth, pmr*)