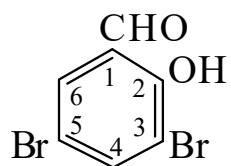




>>Entry Name: 3,5-Dibromo-2-hydroxybenzaldehyde, 9Cl

Synonym(s): 3,5-Dibromosalicylaldehyde, 8Cl



CAS Registry Number: 90-59-5

Related CAS Registry Numbers(s): 61657-65-6

Molecular Formula: C₇H₄Br₂O₂

Molecular Weight: 279.915

Accurate Mass: 277.897802

Percentage Composition: C 30.04%; H 1.44%; Br 57.09%; O 11.43%

Biological Source: Isol. from *Thelepus setosus*

Physical Description: Yellowish prisms

Melting Point: Mp 85 subl.°

pKa Value: pK_{a1} 6.54 (25°, butanol aq.) pK_{a1} 6.17 (25°, H₂O)

Aldrich: 12213-0

>>Derivative: Oxime

CAS Registry Number: 21386-43-6

Molecular Formula: C₇H₅Br₂NO₂

Molecular Weight: 294.93

Accurate Mass: 292.908701

Percentage Composition: C 28.51%; H 1.71%; Br 54.19%; N 4.75%; O 10.85%

Melting Point: Mp 218-220°

>>Derivative: Ac

CAS Registry Number: 109165-13-1

Molecular Formula: C₉H₆Br₂O₃

Molecular Weight: 321.953

Accurate Mass: 319.908367

Percentage Composition: C 33.58%; H 1.88%; Br 49.64%; O 14.91%

Melting Point: Mp 90°

References:

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 124A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 126A, (*ir*)

Lindemann, H. *et al.*, *Annalen*, 1926, **449**, 63-81, (*synth*)

Clarke, K. *et al.*, *J.C.S.*, 1963, 245-250, (*synth*, *pKa*)

Ryabokobylko, Yu.S. *et al.*, *J. Org. Chem. USSR (Engl. Transl.)*, 1974, **10**, 1768, (*pKa*)

Higa, T. *et al.*, *J.A.C.S.*, 1974, **76**, 2246-2248, (*isol*)

Hinterding, K. *et al.*, *Bioorg. Med. Chem.*, 1998, **6**, 1153-1162, (*synth*, *pmr*)

Bandgar, B.P. *et al.*, *Synth. Commun.*, 1998, **28**, 3225-3229, (*synth*)