



>>Entry Name: 2,6-Dichloropyrazine

CAS Registry Number: 4774-14-5

Molecular Formula: C₄H₂Cl₂N₂

Molecular Weight: 148.979

Accurate Mass: 147.959502

Percentage Composition: C 32.25%; H 1.35%; Cl 47.59%; N 18.80%

Melting Point: Mp 57-58° (51-53°)

Boiling Point: Bp₄₀ 120-122°

Aldrich: 13249-7

>>Derivative: 1-Oxide

CAS Registry Number: 61655-70-7

Molecular Formula: C₄H₂Cl₂N₂O

Molecular Weight: 164.978

Accurate Mass: 163.954417

Percentage Composition: C 29.12%; H 1.22%; Cl 42.98%; N 16.98%; O 9.70%

Melting Point: Mp 122-123°

Hazard & Toxicity: Severe skin and eye-irritant

>>Derivative: 4-Oxide

CAS Registry Number: 14399-36-1

Molecular Formula: C₄H₂Cl₂N₂O

Molecular Weight: 164.978

Accurate Mass: 163.954417

Percentage Composition: C 29.12%; H 1.22%; Cl 42.98%; N 16.98%; O 9.70%

Melting Point: Mp 123-125° (119-121°)

Hazard & Toxicity: Severe skin and eye irritant

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 842A; **2**, 842A, (*ir*)

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **3**, 402C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1559C, (*ir*)

Bernardi, L. *et al.*, *Gazz. Chim. Ital.*, 1961, **91**, 1431, (*synth*)

Klein, B. *et al.*, *J.O.C.*, 1963, **28**, 1682, (*synth, uv*)

Noorduyn, L. *et al.*, *Cryst. Struct. Commun.*, 1976, **5**, 153, (*cryst struct*)

Mixan, C.E. *et al.*, *J.O.C.*, 1977, **42**, 1869, (*oxides*)

Morrison, C.A. *et al.*, *J.C.S. Perkin 2*, 1997, 857-868, (*cryst struct*)