



>>Entry Name: 3,6-Pyridazinedicarboxylic acid, 9Cl

CAS Registry Number: 57266-70-3

Molecular Formula: C₆H₄N₂O₄

Molecular Weight: 168.109

Accurate Mass: 168.017108

Percentage Composition: C 42.87%; H 2.40%; N 16.66%; O 38.07%

Physical Description: Pale-yellow cryst. + 2H₂O (H₂O)

Melting Point: Mp 230°

Other Data: Hydrate effloresces at r.t.

>>Derivative: Di-Me ester

CAS Registry Number: 2166-24-7

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: Yellow cryst. (MeOH)

Melting Point: Mp 202°

>>Derivative: Di-Et ester

CAS Registry Number: 113631-50-8

Molecular Formula: C₁₀H₁₂N₂O₄

Molecular Weight: 224.216

Accurate Mass: 224.079708

Percentage Composition: C 53.57%; H 5.39%; N 12.49%; O 28.54%

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 114°

>>Derivative: Dichloride

CAS Registry Number: 187826-59-1

Molecular Formula: C₆H₂Cl₂N₂O₂

Molecular Weight: 204.999

Accurate Mass: 203.949332

Percentage Composition: C 35.15%; H 0.98%; Cl 34.59%; N 13.67%; O 15.61%

Physical Description: Light yellow needles

Melting Point: Mp 208-210 dec.°

>>Derivative: Dihydrazide

CAS Registry Number: 113631-52-0

Molecular Formula: C₆H₈N₆O₂

Molecular Weight: 196.168

Accurate Mass: 196.070874

Percentage Composition: C 36.74%; H 4.11%; N 42.84%; O 16.31%

Physical Description: Yellow cryst.

Melting Point: Mp 290 dec.°

References:

Sueur, S. *et al.*, *J. Het. Chem.*, 1987, **24**, 1285-1289, (*synth, ir, pmr, cmr, cryst struct*)

Fahrni, C.J. *et al.*, *Helv. Chim. Acta*, 1998, **81**, 491-506, (*chloride, synth, ir, pmr, cmr, ms*)