



>>Entry Name: 4,5-Pyridazinedicarboxylic acid

CAS Registry Number: 59648-14-5

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: Plates (EtOAc)

Melting Point: Mp 209-210 dec.°

>>Derivative: Di-Me ester

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: Liq.

>>Derivative: Di-Et ester

CAS Registry Number: 21050-73-7

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: Oil

>>Derivative: Diamide

Molecular Formula: C₆H₆N₄O₂

Molecular Weight: 166.139

Accurate Mass: 166.049076

Percentage Composition: C 43.38%; H 3.64%; N 33.72%; O 19.26%

Physical Description: Cryst.

Melting Point: Mp 249-252°

>>Derivative: Dinitrile

Synonym(s): 4,5-Dicyanopyridazine

CAS Registry Number: 17412-15-6

Molecular Formula: C₆H₂N₄

Molecular Weight: 130.109

Accurate Mass: 130.027946

Percentage Composition: C 55.39%; H 1.55%; N 43.06%

Use/Importance: Synthon for hetero-Diels-Alder reactions

Physical Description: Light yellow needles (EtOH)

Melting Point: Mp 136-137°

>>Derivative: Anhydride

Synonym(s): Furo[3,4-*d*]pyridazine-5,7-dione

CAS Registry Number: 596648-15-6

Molecular Formula: C₆H₂N₂O₃

Molecular Weight: 150.093

Accurate Mass: 150.006543

Percentage Composition: C 48.01%; H 1.34%; N 18.66%; O 31.98%

Melting Point: Mp 184-186 dec.°

References:

- Gabriel, S., *Ber.*, 1903, **36**, 3373-3378, (*synth*)
Raistrick, H. *et al.*, *Biochem. J.*, 1956, **63**, 395-406, (*synth*)
Di Stefano, L. *et al.*, *J. Het. Chem.*, 1968, **5**, 53-59, (*di-Me ester, dinitrile, diamide, synth, ir, uv, pmr*)
Adembri, G. *et al.*, *J.C.S.(C)*, 1968, 2857-2861, (*di-Et ester*)
Turchi, S. *et al.*, *Tetrahedron*, 1997, **53**, 11711-11720, (*dinitrile, use*)
Giomi, D. *et al.*, *J.O.C.*, 2000, **65**, 360-364, (*dinitrile, use, bibl*)