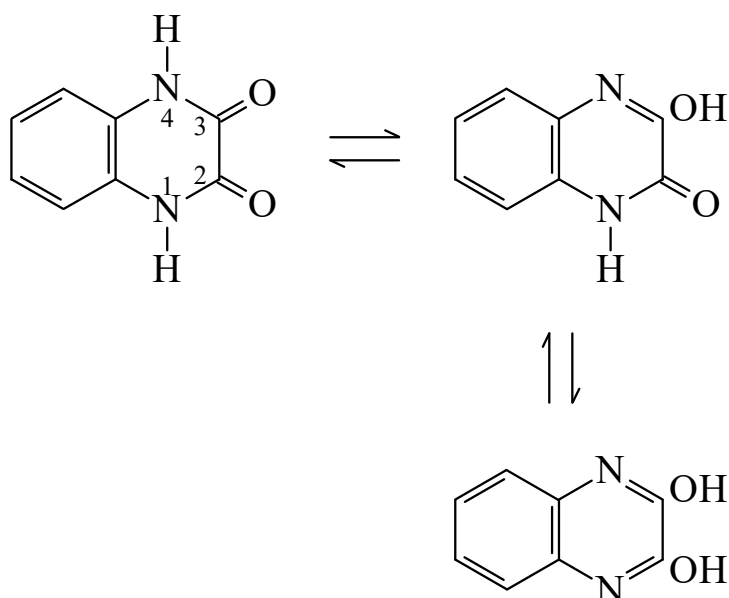




>>Entry Name: 1,4-Dihydro-2,3-quinoxalinedione, 9CI

Synonym(s): 2,3-Quinoxalinediol. 2,3-Dihydroxyquinoxaline. Tetrahydro-2,3-quinoxalinedione



Molecular Formula: C₈H₆N₂O₂

Molecular Weight: 162.148

Accurate Mass: 162.042928

Percentage Composition: C 59.26%; H 3.73%; N 17.28%; O 19.73%

General Statement: Dione form predominates

Physical Description: Needles (H₂O)

Melting Point: Mp 360°

Hazard & Toxicity: LD₅₀ (mus, ipr) 200 mg/kg

>>Derivative: 1-Me

CAS Registry Number: 20934-51-4

Molecular Formula: C₉H₈N₂O₂

Molecular Weight: 176.174

Accurate Mass: 176.058578

Percentage Composition: C 61.36%; H 4.58%; N 15.90%; O 18.16%

Physical Description: Needles (MeNO₂)

Melting Point: Mp 287-288°

>>Variant: Dione-form

CAS Registry Number: 15804-19-0

Molecular Formula: C₈H₆N₂O₂

Molecular Weight: 162.148

Accurate Mass: 162.042928

Percentage Composition: C 59.26%; H 3.73%; N 17.28%; O 19.73%

pKa Value: pK_a 9.52 (20°,H₂O)

Aldrich: 14478-9

Sigma: D3021

>>Derivative: 1,4-Di-Me

CAS Registry Number: 58175-07-8

Molecular Formula: C₁₀H₁₀N₂O₂

Molecular Weight: 190.201

Accurate Mass: 190.074228

Percentage Composition: C 63.15%; H 5.30%; N 14.73%; O 16.82%

Physical Description: Needles (EtOH)

Melting Point: Mp 256-258°

>>Variant: Mono-OH-form

Molecular Formula: C₈H₆N₂O₂

Molecular Weight: 162.148

Accurate Mass: 162.042928

Percentage Composition: C 59.26%; H 3.73%; N 17.28%; O 19.73%