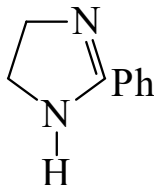




>>Entry Name: 4,5-Dihydro-2-phenyl-1*H*-imidazole, 9Cl

Synonym(s): 2-Phenyl- Δ^2 -imidazoline, 8Cl



CAS Registry Number: 936-49-2

Related CAS Registry Numbers(s): 76902-83-5

Molecular Formula: C₉H₁₀N₂

Molecular Weight: 146.191

Accurate Mass: 146.084398

Percentage Composition: C 73.94%; H 6.89%; N 19.16%

Physical Description: Cryst. (cyclohexane), prisms (C₆H₆) or needles (Me₂CO)

Melting Point: Mp 100-101° (97-99°)

Boiling Point: Bp₅ 162°

pKa Value: p*K*_a 9.9

Aldrich: 21303-9

Fluka: 78727

Sigma: P7271

>>Derivative: Hydrochloride

CAS Registry Number: 7253-39-6

Physical Description: Cryst. (EtOH)

Melting Point: Mp 244°

>>Derivative: Hydroiodide

CAS Registry Number: 56513-57-6

Physical Description: Cryst. (H₂O)

Melting Point: Mp 190°

>>Derivative: Picrate

Melting Point: Mp 242° (233°)

>>Derivative: *N*¹-Benzoyl

Molecular Formula: C₁₆H₁₄N₂O

Molecular Weight: 250.299

Accurate Mass: 250.110613

Percentage Composition: C 76.78%; H 5.64%; N 11.19%; O 6.39%

Melting Point: Mp 99-101°

>>Derivative: *N*¹-Benzoyl; hydrochloride

Melting Point: Mp 169-171°

>>Derivative: *N*¹-4-Methylbenzenesulfonyl

CAS Registry Number: 16054-55-0

Molecular Formula: C₁₆H₁₆N₂O₂S

Molecular Weight: 300.381

Accurate Mass: 300.093248

Percentage Composition: C 63.98%; H 5.37%; N 9.33%; O 10.65%; S 10.68%

Physical Description: Cryst. (Et₂O/EtOH)

Melting Point: Mp 87-89°