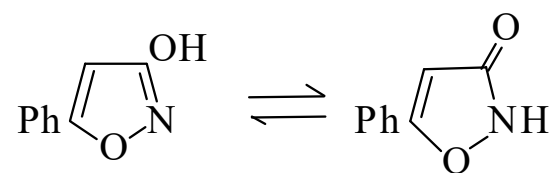




>>Entry Name: 3-Hydroxy-5-phenylisoxazole

Synonym(s): 5-Phenyl-3(2*H*)-isoxazolone, 9Cl. 5-Phenyl-3-isoxazolol, 8Cl



CAS Registry Number: 939-05-9

Extra CAS Registry Numbers(s): 32306-29-9

Molecular Formula: C₉H₇NO₂

Molecular Weight: 161.16

Accurate Mass: 161.047679

Percentage Composition: C 67.08%; H 4.38%; N 8.69%; O 19.86%

Physical Description: Cryst. (MeOH or hexane)

Melting Point: Mp 164-165°

Boiling Point: Subl. 140°

UV: [neutral] λ_{max} 262 (19500) (cyclohexane)

Other Data: Dimorphous

>>Derivative: Me ether

Synonym(s): 3-Methoxy-5-phenylisoxazole

CAS Registry Number: 942-68-7

Molecular Formula: C₁₀H₉NO₂

Molecular Weight: 175.187

Accurate Mass: 175.063329

Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%

Physical Description: Cryst. (hexane)

Melting Point: Mp 69-70°

>>Derivative: Et ether

CAS Registry Number: 23244-34-0

Molecular Formula: C₁₁H₁₁NO₂

Molecular Weight: 189.213

Accurate Mass: 189.078979

Percentage Composition: C 69.83%; H 5.86%; N 7.40%; O 16.91%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 35°

References:

- Pierfrancesco, B. *et al.*, *Gazz. Chim. Ital.*, 1961, **91**, 47-64; 1966, **96**, 454-464, (*synth*)
Boulton, A.J. *et al.*, *Tetrahedron*, 1964, **20**, 2835, (*synth*)
Iwai, I. *et al.*, *Chem. Pharm. Bull.*, 1966, **14**, 1277, (*synth*)
Biagini, S. *et al.*, *Acta Cryst. B*, 1969, **25**, 2108, (*cryst struct*)
Sørensen, U.S. *et al.*, *J.O.C.*, 2000, **65**, 1003-1007, (*synth, pmr, cmr*)