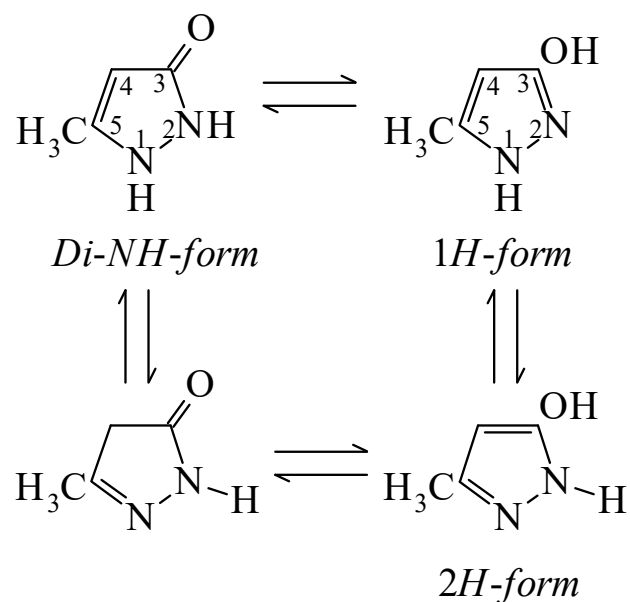




>>Entry Name: 3(5)-Hydroxy-5(3)-methylpyrazole

Synonym(s): 1,2-Dihydro-5-methyl-3*H*-pyrazol-3-one, 9CI. 3-Methyl-3-pyrazolin-5-one. 5(3)-Methyl-3(5)-pyrazolol. 3-Methyl-5-pyrazolone



CAS Registry Number: 4344-87-0

Extra CAS Registry Numbers(s): 108-26-9

Molecular Formula: C₄H₆N₂O

Molecular Weight: 98.104

Accurate Mass: 98.048013

Percentage Composition: C 48.97%; H 6.16%; N 28.55%; O 16.31%

Physical Description: Cryst. (DMF), microcryst. mass (other solvs.)

Melting Point: Mp 215°

Aldrich: 30306-2

>>Derivative: *N*¹-Ac

CAS Registry Number: 52182-91-9

Molecular Formula: C₆H₈N₂O₂

Molecular Weight: 140.141

Accurate Mass: 140.058578

Percentage Composition: C 51.42%; H 5.75%; N 19.99%; O 22.83%

Physical Description: Needles

Melting Point: Mp 140°

>>Derivative: *N*¹-Me

Synonym(s): 3-Hydroxy-1,5-dimethyl-1*H*-pyrazole. 1,2-Dihydro-1,5-dimethyl-3*H*-pyrazol-3-one. 1,5-Dimethyl-3-pyrazolone

CAS Registry Number: 3201-28-3

Molecular Formula: C₅H₈N₂O

Molecular Weight: 112.131

Accurate Mass: 112.063663

Percentage Composition: C 53.56%; H 7.19%; N 24.98%; O 14.27%

Melting Point: Mp 172-173°

Other Data: *OH*-Form predominates, but *N*(2)*H*-form is important in polar media

>>Derivative: *N*²-Me

Synonym(s): 5-Hydroxy-1,3-dimethyl-1*H*-pyrazole. 2,4-Dihydro-2,5-dimethyl-3*H*-pyrazol-3-one. 1,3-Dimethyl-5-pyrazolone. 2,5-Dimethyl-3-pyrazolinone

CAS Registry Number: 2749-59-9

Molecular Formula: C₅H₈N₂O

Molecular Weight: 112.131

Accurate Mass: 112.063663

Percentage Composition: C 53.56%; H 7.19%; N 24.98%; O 14.27%

Physical Description: Cryst. (CHCl₃)

Melting Point: Mp 100-105° (122-123.5°)

pK_a Value: pK_a 7.94

Other Data: *N*(1)*H*-Form predominates in polar, *C*(4)*H*-form in nonpolar media