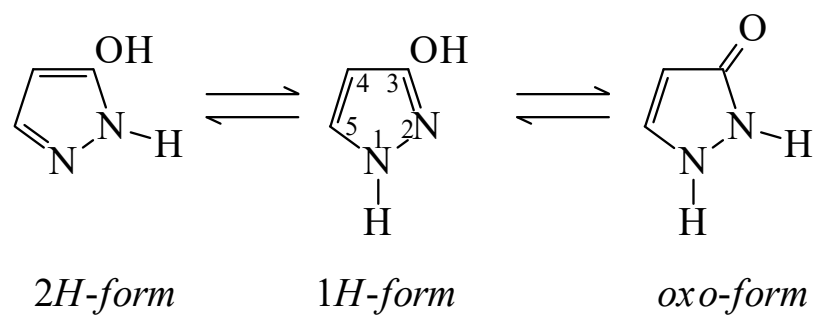




>>Entry Name: 3(5)-Pyrazolol

Synonym(s): 1,2-Dihydro-3*H*-pyrazol-3-one. 3-Pyrazolinone. 3(5)-Hydroxypyrazole. 2-Pyrazolin-5-one. 5-Pyrazolone



CAS Registry Number: 137-45-1

Related CAS Registry Numbers(s): 10234-66-9

Extra CAS Registry Numbers(s): 39455-90-8

Molecular Formula: C<sub>3</sub>H<sub>4</sub>N<sub>2</sub>O

Molecular Weight: 84.077

Accurate Mass: 84.032363

Percentage Composition: C 42.86%; H 4.80%; N 33.32%; O 19.03%

Use/Importance: Intermed. for dyes and pharmaceuticals

Physical Description: Cryst. (H<sub>2</sub>O or toluene)

Melting Point: Mp 166°

Solubility: Sol. H<sub>2</sub>O

Other Data: Sublimes

>>Variant: 1*H*-form

Molecular Formula: C<sub>3</sub>H<sub>4</sub>N<sub>2</sub>O

Molecular Weight: 84.077

Accurate Mass: 84.032363

Percentage Composition: C 42.86%; H 4.80%; N 33.32%; O 19.03%

>>Derivative: 1-Me

Synonym(s): 1,2-Dihydro-1-methyl-3*H*-pyrazol-3-one. 3-Hydroxy-1-methylpyrazole

CAS Registry Number: 52867-35-3

Molecular Formula: C<sub>4</sub>H<sub>6</sub>N<sub>2</sub>O

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. (toluene)

Melting Point: Mp 128°

>>Derivative: 1-Ph

Synonym(s): 3-Hydroxy-1-phenylpyrazole. 1-Phenyl-1*H*-pyrazol-3-ol

CAS Registry Number: 1008-79-3

Molecular Formula: C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O

Molecular Weight: 160.175

Accurate Mass: 160.063663

Percentage Composition: C 67.49%; H 5.03%; N 17.49%; O 9.99%

Physical Description: Needles (H<sub>2</sub>O)

Melting Point: Mp 153-155°. Mp 111° (as hydrochloride)

pKa Value: p*K*<sub>a1</sub> 0.46; p*K*<sub>a2</sub> 7.72

>>Derivative: 1-Ph, *O*-Ac

Molecular Formula: C<sub>11</sub>H<sub>10</sub>N<sub>2</sub>O<sub>2</sub>

Molecular Weight: 202.212

Accurate Mass: 202.074228

Percentage Composition: C 65.34%; H 4.98%; N 13.85%; O 15.82%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 66-67°