



Synonym(s): 1,2-Dihydro-2-methyl-5-(trifluoromethyl)-3*H*-pyrazol-3-one, 9Cl. 3-Hydroxy-2-methyl-5-(trifluoromethyl)pyrazole. 1-Methyl-3-(trifluoromethyl)-5-pyrazolinone. 5-Hydroxy-1-methyl-3-(trifluoromethyl)pyrazole

CAS Registry Number: 122431-37-2

Molecular Formula: C₅H₅F₃N₂O

Molecular Weight: 166.102

Accurate Mass: 166.035397

Percentage Composition: C 36.16%; H 3.03%; F 34.31%; N 16.87%; O 9.63%

Use/Importance: Aldehyde scavenger used in colour photographic materials

Physical Description: Prisms (HCl aq. or Et₂O/petrol)

Melting Point: Mp 174-175.5°

>>Derivative: *N*-Benzyl

CAS Registry Number: 143706-79-0

Molecular Formula: C₁₁H₉F₃N₂O

Molecular Weight: 242.2

Accurate Mass: 242.066697

Percentage Composition: C 54.55%; H 3.75%; F 23.53%; N 11.57%; O 6.61%

Physical Description: Solid

Melting Point: Mp 224.5-225.5°

>>Derivative: *N*-Ph

Molecular Formula: C₁₀H₇F₃N₂O

Molecular Weight: 228.173

Accurate Mass: 228.051047

Percentage Composition: C 52.64%; H 3.09%; F 24.98%; N 12.28%; O 7.01%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 185-187°

References:

Gilman, H. *et al.*, *J.A.C.S.*, 1946, **68**, 426, (*synth*)

De Stevens, G. *et al.*, *J.A.C.S.*, 1959, **81**, 6292, (*derivs*)

Atherton, J.H. *et al.*, *J.C.S.(C)*, 1968, 1507, (*synth, pmr, F-19 nmr*)

Poulter, C.D. *et al.*, *J.O.C.*, 1981, **46**, 1532, (*synth, pmr, ir, ms*)

Lee, L.F. *et al.*, *J. Het. Chem.*, 1990, **27**, 243, (*N-Me derivs, synth, pmr, cmr, F-19 nmr, ir*)

Hamper, B.C. *et al.*, *J.O.C.*, 1992, **57**, 5680, (*derivs, synth, cmr, F-19 nmr, glc*)