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>>Entry Name: 4-Nitropyrazole

CAS Registry Number: 2075-46-9

Molecular Formula:  $C_3H_3N_3O_2$

Molecular Weight: 113.076

Accurate Mass: 113.022527

Percentage Composition: C 31.87%; H 2.67%; N 37.16%; O 28.30%

Physical Description: Needles ( $C_6H_6$ )

Melting Point: Mp 162°

Boiling Point: Bp 323°

pKa Value:  $pK_a -1.96$  (20°,  $H_2SO_4$  aq.)

Rare Chemicals Library: S93940-4

>>Derivative: 1-Nitro

Synonym(s): 1,4-Dinitro-1*H*-pyrazole, 9CI

CAS Registry Number: 35852-77-8

Molecular Formula:  $C_3H_2N_4O_4$

Molecular Weight: 158.073

Accurate Mass: 158.007606

Percentage Composition: C 22.80%; H 1.28%; N 35.44%; O 40.49%

Physical Description: Cryst. (hexane)

Melting Point: Mp 54°

References:

Hüttel, R. *et al.*, *Chem. Ber.*, 1955, **88**, 1577

Buchanan, J.G. *et al.*, *J.C.S. Perkin 1*, 1989, 925, (1-nitro)