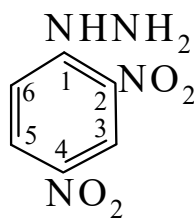




>>Entry Name: (2,4-Dinitrophenyl)hydrazine, 9Cl, 8Cl

Synonym(s): DNPH. Brady's reagent



CAS Registry Number: 119-26-6

Type of Compound Code(s): PS7850 PG5500 PG5150

Molecular Formula: C₆H₆N₄O₄

Molecular Weight: 198.138

Accurate Mass: 198.038906

Percentage Composition: C 36.37%; H 3.05%; N 28.28%; O 32.30%

Use/Importance: Reagent for characterisation of carbonyl compds.; also effects dehydrohalogenation of α -halogeno ketones etc. Acid-base indicator (pH range: 7.6-9.6; colour change: red $\rightarrow$ yellow)

Physical Description: Blue-red cryst. with violet fluor.

Melting Point: Mp 198 dec. $^{\circ}$ (194 $^{\circ}$)

pKa Value: pK_a 9.1 (25 $^{\circ}$)

Hazard & Toxicity: Eye and skin irritant. Symptoms of exposure can be delayed. Can cause methaemoglobinaemia. LD₅₀ 654 mg/kg. Potential mutagen

Aldrich: D19930-3

Fluka: 42210

Sigma: D2630

>>Derivative: N-Ac

Molecular Formula: C₈H₈N₄O₅

Molecular Weight: 240.175

Accurate Mass: 240.049471

Percentage Composition: C 40.01%; H 3.36%; N 23.33%; O 33.31%

Physical Description: Yellow needles (EtOH aq.)

Melting Point: Mp 197-198 $^{\circ}$

>>Derivative: N-Benzoyl

Molecular Formula: C₁₃H₁₀N₄O₅

Molecular Weight: 302.246

Accurate Mass: 302.065121

Percentage Composition: C 51.66%; H 3.33%; N 18.54%; O 26.47%

Physical Description: Orange-red leaflets (EtOH)

Melting Point: Mp 206-207 $^{\circ}$

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **2**, 752C, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1371D, (ir)

Org. Synth., Coll. Vol., 2, 1943, 228, (synth)

Murashova, V.I. et al., Zh. Anal. Khim., 1964, **19**, 1503, (use)

Ault, A., J. Chem. Educ., 1965, **42**, 267, (synth)

Legradi, L., Magy. Kem. Foly., 1965, **71**, 302, (use)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 176

Buckingham, J., Q. Rev., Chem. Soc., 1969, **23**, 37, (rev)

Pearson, D.E., Org. Prep. Proced. Int., 1972, **4**, 49, (synth)

Keiser, J.K., J. Chem. Educ., 1974, **51**, 599, (pmr)

Allen, C.F.H., Can. J. Chem., 1975, **53**, 865, (ms)

Okabe, N. et al., Acta Cryst. C, 1993, **49**, 1678, (cryst struct, tox)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, DVC400

Luxon, S.G., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry, 1992, 539