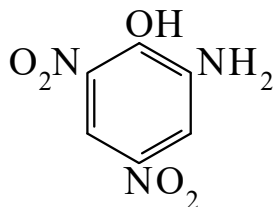




>>Entry Name: **2-Amino-4,6-dinitrophenol**, 9CI

Synonym(s): 2-Hydroxy-3,5-dinitroaniline. Picramic acid. Picraminic acid



CAS Registry Number: 96-91-3

Related CAS Registry Numbers(s): 831-52-7

Molecular Formula: C₆H₅N₃O₅

Molecular Weight: 199.123

Accurate Mass: 199.022922

Percentage Composition: C 36.19%; H 2.53%; N 21.10%; O 40.17%

Use/Importance: Intermediate for azo dyestuffs. Used as a 0.1% soln. in EtOH for photometric detn. of Au(III), Ce(IV), Fe(III), V(V)

Physical Description: Dark-red needles (EtOH), prisms (CHCl₃)

Melting Point: Mp 169°

Solubility: Sol. EtOH, C₆H₆; v. spar. sol. H₂O

pKa Value: pK_a 4.7

Hazard & Toxicity: Explosive when dry

Rare Chemicals Library: S50885-3

>>Derivative: *N*-Ac

CAS Registry Number: 5422-72-0

Molecular Formula: C₈H₇N₃O₆

Molecular Weight: 241.16

Accurate Mass: 241.033487

Percentage Composition: C 39.84%; H 2.93%; N 17.42%; O 39.81%

Physical Description: Needles (H₂O)

Melting Point: Mp 201°

>>Derivative: *N*-Benzoyl

Molecular Formula: C₁₃H₉N₃O₆

Molecular Weight: 303.231

Accurate Mass: 303.049137

Percentage Composition: C 51.49%; H 2.99%; N 13.86%; O 31.66%

Physical Description: Greenish-yellow needles (AcOH or xylene)

Melting Point: Mp 299-300°

>>Derivative: *N*-(4-Methylbenzenesulfonyl)

Molecular Formula: C₁₃H₁₁N₃O₇S

Molecular Weight: 353.312

Accurate Mass: 353.031772

Percentage Composition: C 44.19%; H 3.14%; N 11.89%; O 31.70%; S 9.08%

Melting Point: Mp 191°

>>Derivative: *O*-Ac

Molecular Formula: C₈H₇N₃O₆

Molecular Weight: 241.16

Accurate Mass: 241.033487

Percentage Composition: C 39.84%; H 2.93%; N 17.42%; O 39.81%

Melting Point: Mp 193°

>>Derivative: *O*-Benzoyl

Molecular Formula: C₁₃H₉N₃O₆

Molecular Weight: 303.231

Accurate Mass: 303.049137

Percentage Composition: C 51.49%; H 2.99%; N 13.86%; O 31.66%

Melting Point: Mp 218-219°