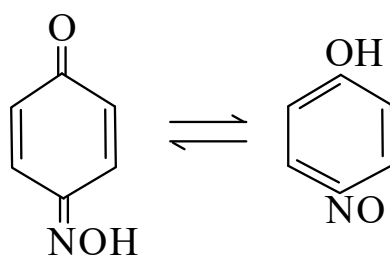




>>Entry Name: 4-Nitrosophenol

Synonym(s): 2,5-Cyclohexadiene-1,4-dione monoxime, 9CI. 1,4-Benzoquinone monoxime



CAS Registry Number: 637-62-7

Extra CAS Registry Numbers(s): 104-91-6

Molecular Formula: C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub>

Molecular Weight: 123.111

Accurate Mass: 123.032029

Percentage Composition: C 58.54%; H 4.09%; N 11.38%; O 25.99%

Physical Description: Pale yellow cryst. (Et<sub>2</sub>O)

Melting Point: Mp 126-128°. Mp 137 dec.°

pK<sub>a</sub> Value: pK<sub>a</sub> 6.48 (25°)

Hazard & Toxicity: Can ignite spontaneously on storage if impure. Irritant.

>>Variant: Oxime-form

Molecular Formula: C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub>

Molecular Weight: 123.111

Accurate Mass: 123.032029

Percentage Composition: C 58.54%; H 4.09%; N 11.38%; O 25.99%

>>Derivative: O-Me

Synonym(s): *p*-Benzoquinone monoxime methyl ether

CAS Registry Number: 15312-05-7

Molecular Formula: C<sub>7</sub>H<sub>7</sub>NO<sub>2</sub>

Molecular Weight: 137.138

Accurate Mass: 137.047679

Percentage Composition: C 61.31%; H 5.14%; N 10.21%; O 23.33%

Physical Description: Golden needles (petrol)

Melting Point: Mp 83°

>>Variant: Nitroso-form

Molecular Formula: C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub>

Molecular Weight: 123.111

Accurate Mass: 123.032029

Percentage Composition: C 58.54%; H 4.09%; N 11.38%; O 25.99%

>>Derivative: Me ether

Synonym(s): 1-Methoxy-4-nitrosobenzene, 9CI. *p*-Nitrosoanisole

CAS Registry Number: 1516-21-8

Molecular Formula: C<sub>7</sub>H<sub>7</sub>NO<sub>2</sub>

Molecular Weight: 137.138

Accurate Mass: 137.047679

Percentage Composition: C 61.31%; H 5.14%; N 10.21%; O 23.33%

Physical Description: Bluish-green prisms (petrol)

Melting Point: Mp 23°

>>Derivative: Et ether

Synonym(s): 1-Ethoxy-4-nitrosobenzene, 9CI. *p*-Nitrosophenetole