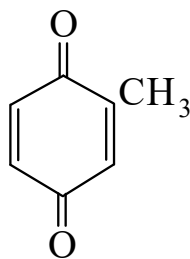




>>Entry Name: 2-Methyl-1,4-benzoquinone

ENTRY UNDER REVIEW

Synonym(s): 2-Methyl-2,5-cyclohexadiene-1,4-dione, 9CI. Methylquinone. *p*-Toluquinone. Toluquinone



CAS Registry Number: 553-97-9

Molecular Formula: C<sub>7</sub>H<sub>6</sub>O<sub>2</sub>

Molecular Weight: 122.123

Accurate Mass: 122.03678

Percentage Composition: C 68.85%; H 4.95%; O 26.20%

Biological Source: Component of arthropod defensive secretions

Physical Description: Yellow plates or needles

Melting Point: Mp 69°

Solubility: BERDY SOL: Sol. MeOH, hexane; poorly sol. H<sub>2</sub>O

UV: [neutral] λ<sub>max</sub> 249 (ε 21380); 255 (ε 18620); 315 (ε 630); 436 (ε 24) (CHCl<sub>3</sub>) (Berdy)

Other Data: Sublimes. Steam-volatile

Hazard & Toxicity: Skin irritant

Aldrich: 21131-1

Fluka: 89590

Rare Chemicals Library: S57121-0

>>Derivative: 1-Oxime

Synonym(s): 3-Methyl-4-nitrosophenol. 4-Nitroso-*m*-cresol

CAS Registry Number: 13362-34-0

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: Needles (H<sub>2</sub>O or C<sub>6</sub>H<sub>6</sub>), prisms (AcOH)

Melting Point: Mp 156°. Mp 165°

pKa Value: pK<sub>a1</sub> 6.95

>>Derivative: 4-Oxime

Synonym(s): 2-Methyl-4-nitrosophenol. 4-Nitroso-*o*-cresol

CAS Registry Number: 13362-33-9

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: Needles (Et<sub>2</sub>O/petrol)

Melting Point: Mp 134-135°

>>Derivative: Dioxime

CAS Registry Number: 36164-91-7

Molecular Formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>

Molecular Weight: 152.152

Accurate Mass: 152.058578

Percentage Composition: C 55.26%; H 5.30%; N 18.41%; O 21.03%

Physical Description: Needles

Melting Point: Mp 234 dec.°

>>Derivative: Bis-2,4-dinitrophenylhydrazone

Physical Description: Greyish-black needles (PhNO<sub>2</sub>)

Melting Point: Mp 269°