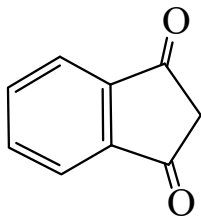




>>Entry Name: **1,3-Indanedione**

Synonym(s): 1,3-Dioxohydrindene



CAS Registry Number: 606-23-5

Molecular Formula: C<sub>9</sub>H<sub>6</sub>O<sub>2</sub>

Molecular Weight: 146.145

Accurate Mass: 146.03678

Percentage Composition: C 73.97%; H 4.14%; O 21.90%

Physical Description: Needles (petrol)

Melting Point: Mp 130-131°

Solubility: Spar. sol. H<sub>2</sub>O, sol. hot EtOH, C<sub>6</sub>H<sub>6</sub>

pK<sub>a</sub> Value: pK<sub>a</sub> 7.2 (20°, 1% EtOH)

Other Data: Deep-yellow soln. in alkali (enol form)

**Hazard & Toxicity:** Exp. reprod. and teratogenic effects

Aldrich: I-200-2

Fluka: 56860

>>Derivative: Dioxime

CAS Registry Number: 6624-48-2

Molecular Formula: C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>

Molecular Weight: 176.174

Accurate Mass: 176.058578

Percentage Composition: C 61.36%; H 4.58%; N 15.90%; O 18.16%

Melting Point: Mp 220-225 dec.°

>>Derivative: Phenylhydrazone

Melting Point: Mp 162-163°

>>Derivative: Bisphenylhydrazone

Physical Description: Pink needles

Melting Point: Mp 171°

>>Derivative: Bis(thiosemicarbazone)

Synonym(s): 2,2'-(1*H*-Indene-1,3(2*H*)-diylidene)bishydrazinecarbothioamide, 9CI

CAS Registry Number: 3401-45-4

Molecular Formula: C<sub>11</sub>H<sub>12</sub>N<sub>6</sub>S<sub>2</sub>

Molecular Weight: 292.388

Accurate Mass: 292.056484

Percentage Composition: C 45.19%; H 4.14%; N 28.74%; S 21.93%

Use/Importance: Used as 0.8% DMF soln. for photometric detn. of IO<sub>4</sub><sup>(-)</sup> (λ<sub>max</sub> 520 nm, ε 4800, pH 1.7-2.5)

Physical Description: Grey powder (Py aq.)

Melting Point: Mp 236-242 dec.°

Solubility: Sol. Py, DMF; insol. H<sub>2</sub>O, EtOH, Et<sub>2</sub>O, C<sub>6</sub>H<sub>6</sub>

#### References:

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 881A, (*nmr*)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 54D, (*ir*)

Horn, O. *et al.*, *Chem. Ber.*, 1951, **84**, 607

Grinsteins, V. *et al.*, *Zh. Obshch. Khim.*, 1962, **32**, 1077, (*synth*)

Norcross, B.E., *J. Chem. Educ.*, 1965, **42**, 268

Bravic, G. *et al.*, *Cryst. Struct. Commun.*, 1976, **5**, 1, (*cryst struct*)

Hughes, D.W. *et al.*, *Can. J. Chem.*, 1977, **55**, 3304, (*cmr*)

Shapiro, B.L. *et al.*, *J. Phys. Chem. Ref. Data*, 1977, **6**, 919