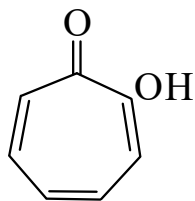




>>Entry Name: Tropolone, 8Cl

Synonym(s): 2-Hydroxy-2,4,6-cycloheptatrien-1-one, 9Cl



CAS Registry Number: 533-75-5

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: Isol. from *Pseudomonas plantari*

Use/Importance: Used as 0.01M aq. soln. for photometric detn. of Ru(III) ( $\lambda_{\text{max}}$  415 nm,  $\epsilon$  18700), Rh(III), Cr(III)

Physical Description: Needles (hexane or petrol)

Melting Point: Mp 49-50°

Solubility: Sol. H<sub>2</sub>O; v. sol. org. solvs. except hydrocarbons

pKa Value: pK<sub>a1</sub> -0.53; pK<sub>a2</sub> 6.67 (25°, OH, 0.5M NaCl)

Other Data: Amphoteric. Forms a yellow anion in alkaline soln.. Sol. unchanged in conc. HCl

Hazard & Toxicity: LD<sub>50</sub> (rat, ipr) 190 mg/kg

Aldrich: T8970-2

Fluka: 93555

Rare Chemicals Library: S3667-7

Sigma: T7387

>>Derivative: Hydrochloride

Physical Description: Clusters of needles (HCl/MeOH)

Melting Point: Mp 131-132° (gas evolution, softens at 114-115°)

Other Data: Dec. slowly at r.t.

>>Derivative: Picrate

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 119-120° (83.5-84°)

>>Derivative: Ac

Synonym(s): 2-(Acetyloxy)-2,4,6-cycloheptatrien-1-one, 9Cl

CAS Registry Number: 33739-54-7

Molecular Formula: C<sub>9</sub>H<sub>8</sub>O<sub>3</sub>

Molecular Weight: 164.16

Accurate Mass: 164.047345

Percentage Composition: C 65.85%; H 4.91%; O 29.24%

Physical Description: Cryst. (cyclohexane)

Melting Point: Mp 80° (67°)

>>Derivative: Benzoyl

Synonym(s): 2-Benzoyloxy-2,4,6-cycloheptatrien-1-one, 9Cl

CAS Registry Number: 58244-35-2

Molecular Formula: C<sub>14</sub>H<sub>10</sub>O<sub>3</sub>

Molecular Weight: 226.231

Accurate Mass: 226.062995

Percentage Composition: C 74.33%; H 4.46%; O 21.22%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 129-130°