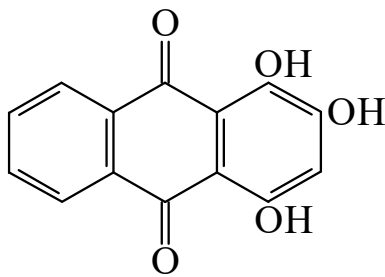




>>Entry Name: 1,2,4-Trihydroxyanthraquinone

Synonym(s): 1,2,4-Trihydroxy-9,10-anthracenedione, 9CI. **Purpurin**‡. Madder purple. Verantin. Oxylizarinic acid



CAS Registry Number: 81-54-9

Molecular Formula: C<sub>14</sub>H<sub>8</sub>O<sub>5</sub>

Molecular Weight: 256.214

Accurate Mass: 256.037175

Percentage Composition: C 65.63%; H 3.15%; O 31.22%

Biological Source: Found in madder root as glucoside, common plant pigment. Isol. from tissue cultures of *Galium mollugo* and *Cinchona ledgeriana*

Use/Importance: Used as textile dye. Used as 0.4mM soln. in 4-methyl-2-pentanone for extraction-photometric detn. of Ge and Fe (III) ( $\lambda_{\max}$  595 nm)

Physical Description: Long orange-red or orange-yellow needles + 1H<sub>2</sub>O (EtOH aq.), dark-red needles (EtOH)

Melting Point: Mp 259°

Solubility: Spar. sol. hot H<sub>2</sub>O

UV: [neutral]  $\lambda_{\max}$  255 (); 485 (); 518 () (MeOH) (Berdy) [neutral]  $\lambda_{\max}$  255 ( $\epsilon$  25600); 485 ( $\epsilon$  8300); 518 ( $\epsilon$  7400) (EtOH) (Berdy)

Other Data: Sol. H<sub>2</sub>SO<sub>4</sub>, alkalis → red solns. Forms cryst. Na, K, Pb salts

Hazard & Toxicity: Eye irritant

Aldrich: 22914-8

Fluka: 82631

Rare Chemicals Library: S44351-4

Sigma: P0274

>>Derivative: 2,4-Di-Ac

Molecular Formula: C<sub>18</sub>H<sub>12</sub>O<sub>7</sub>

Molecular Weight: 340.289

Accurate Mass: 340.058305

Percentage Composition: C 63.53%; H 3.55%; O 32.91%

Melting Point: Mp 175-178°

>>Derivative: Tri-Ac

CAS Registry Number: 10228-14-5

Molecular Formula: C<sub>20</sub>H<sub>14</sub>O<sub>8</sub>

Molecular Weight: 382.326

Accurate Mass: 382.06887

Percentage Composition: C 62.83%; H 3.69%; O 33.48%

Physical Description: Pale yellow needles

Melting Point: Mp 198-200°

Other Data: Sinters at 193°

>>Derivative: 1-Me ether

Synonym(s): 2,4-Dihydroxy-1-methoxyanthraquinone. Purpurin 1-methyl ether

CAS Registry Number: 94099-66-8

Molecular Formula: C<sub>15</sub>H<sub>10</sub>O<sub>5</sub>

Molecular Weight: 270.241

Accurate Mass: 270.052825

Percentage Composition: C 66.67%; H 3.73%; O 29.60%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 230°

Other Data: Formerly descr. as isol. from *Cinchona ledgeriana* and *Cinchona pubescens*. Assignment revised in 1996