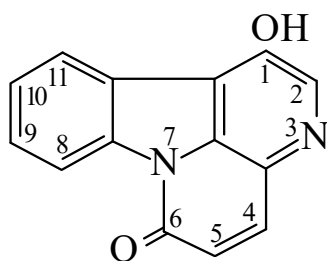




>>Entry Name: 1-Hydroxycanthin-6-one

Synonym(s): 1-Hydroxy-6*H*-indolo[3,2,1-*de*][1,5]naphthyridin-6-one, 9CI



CAS Registry Number: 80787-59-3

Molecular Formula: C<sub>14</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>

Molecular Weight: 236.229

Accurate Mass: 236.058578

Percentage Composition: C 71.18%; H 3.41%; N 11.86%; O 13.55%

Biological Source: Alkaloid from the heartwood of *Ailanthus giraldii* and root bark of *Ailanthus altissima* (Simaroubaceae)

Physical Description: Yellow cryst. (MeOH/Me<sub>2</sub>CO)

Melting Point: Mp 220°

>>Derivative: Ac

Molecular Formula: C<sub>16</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>

Molecular Weight: 278.267

Accurate Mass: 278.069143

Percentage Composition: C 69.06%; H 3.62%; N 10.07%; O 17.25%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 205°

>>Derivative: Me ether

Synonym(s): 1-Methoxycanthin-6-one. 1-Methoxy-6*H*-indolo[3,2,1-*de*][1,5]naphthyridin-6-one, 9CI

CAS Registry Number: 60755-86-4

Molecular Formula: C<sub>15</sub>H<sub>10</sub>N<sub>2</sub>O<sub>2</sub>

Molecular Weight: 250.256

Accurate Mass: 250.074228

Percentage Composition: C 71.99%; H 4.03%; N 11.19%; O 12.79%

Biological Source: Alkaloid from the wood and root bark of *Ailanthus altissima*, and from the root bark of *Ailanthus excelsa* (Simaroubaceae)

Use/Importance: Cytotoxic to guinea pig keratocytes

Physical Description: Pale-yellow needles (Me<sub>2</sub>CO or MeOH)

Melting Point: Mp 250-250.5° (246°)

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

UV: [neutral] λ<sub>max</sub> 259 (); 270 (); 280 (); 346 (); 360 (); 383 () (MeOH) (Berdy) [neutral] λ<sub>max</sub> 279 (ε 12300); 330 (ε 7500); 361 (ε 17400); 370 (ε 16300); 378 (ε 19000) (EtOH) (Berdy)

>>Derivative: Me ether, *N*-oxide

Synonym(s): 1-Methoxycanthin-6-one *N*(3)-oxide

CAS Registry Number: 77370-00-4

Molecular Formula: C<sub>15</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>

Molecular Weight: 266.256

Accurate Mass: 266.069143

Percentage Composition: C 67.67%; H 3.79%; N 10.52%; O 18.03%

Biological Source: Alkaloid from the root bark of *Ailanthus altissima* (Simaroubaceae)

Physical Description: Yellow needles (CHCl<sub>3</sub>)

Melting Point: Mp 256-257°

References:

- Ohmoto, T. *et al.*, *Chem. Pharm. Bull.*, 1976, **24**, 1532, (*isol, uv, ir, pmr, ms, struct*)  
Cordell, G.A. *et al.*, *J. Nat. Prod.*, 1978, **41**, 166, (*isol*)  
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Varga, E. *et al.*, *Fitoterapia*, 1981, **52**, 183, (*isol*)  
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