

## Product Information

### Crotaline

**Cat. No.:** X23-04-XQ444

**Size:** 20 mg; 50 mg; 100 mg; 200 mg

**MDL:** MFCD00084656

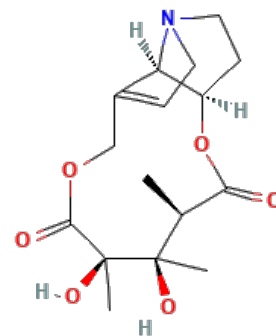
**CAS Number:** 315-22-0

**Compound CID:** 9415

**Synonym:** 315-22-0; Monocrotaline; Crotaline; Monocrotalin; (-)-Monocrotaline;

Retronecine cyclic 2,3-dihydroxy-2,3,4-trimethylglutarate;

(13- $\alpha$ ,14- $\alpha$ )-14,19-Dihydro-12,13-dihydroxy-20-norcrotalanan-11,15-dione



**This product is for research use only and is not intended for diagnostic use.**

### Product Information

<b>Description</b>	Crotaline is an pyrrolizidine alkaloid that induce pulmonary hypertension in rodents.
<b>Molecular Weight</b>	325.36
<b>Molecular Formula</b>	C <sub>16</sub> H <sub>23</sub> NO <sub>6</sub>
<b>IUPAC Name</b>	(1 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>R</i> ,16 <i>R</i> ) )-5,6-Dihydroxy-4,5,6-trimethyl-2,8-dioxa-13-azatricyclo[8.5.1.0 <sup>13,16</sup> ]hexadec-10-ene-3,7-dione
<b>InChI</b>	InChI=1S/C16H23NO6/c1-9-13(18)23-11-5-7-17-6-4-10(12(11)17)8-22-14(19)16(3,21)15(9,2)20/h4,9,11-12,20-21H,5-8H2,1-3H3/t9-,11+,12+,15+,16-/m0/s1
<b>InChI Key</b>	QVCMHGGNRFMAD-XFGHUUIASA-N
<b>Canonical SMILES</b>	CC1C(=O)OC2CCN3C2C(=CC3)COC(=O)C(C1(C)O)(C)O
<b>Isomeric SMILES</b>	C[C@H]1C(=O)O[C@@H]2CCN3[C@@H]2C(=CC3)COC(=O)[C@]1([C@]1(C)O)(C)O
<b>Source</b>	<i>Legume showy crotalaria</i>
<b>Form</b>	White prismatic crystal
<b>Purity</b>	>98%, determined by HPLC.
<b>Solubility</b>	It is slightly soluble in water, soluble in methanol and absolute ethanol, and easily soluble in chloroform.
<b>Identity</b>	Confirmed by NMR and MS.
<b>Stability</b>	The product is stable for two years when stored at the recommended temperature.
<b>Melting Point</b>	196~198°C
<b>Applications</b>	Crotaline can be used for anticancer activity experiments, etc.



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**Storage**

Store at 4°C. Protect from light.

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**Safety Information**

**Personal Protective**

Gloves, eyeshields, N95 mask

**Equipment**

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