

## Product Information

### CB1954, Purity ≥98%

**Cat. No.:** X24-09-YM1361

**Size:** 10 mg; 25 mg; 50 mg; 100 mg

**MDL:** MFCD00869490

**CAS Number:** 21919-05-1

**Compound CID:** 89105

**Synonym:** 21919-05-1; Tretazicar; 5-(Aziridin-1-yl)-2,4-dinitrobenzamide

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



### Product Information

<b>Description</b>	CB1954, soluble in DMSO and insoluble in water and ethanol, is an anticancer compound. The molecular weight of the compound is 252.18, and its molecular formula is C <sub>9</sub> H <sub>8</sub> N <sub>4</sub> O <sub>5</sub> .
<b>Molecular Weight</b>	252.18
<b>Molecular Formula</b>	C <sub>9</sub> H <sub>8</sub> N <sub>4</sub> O <sub>5</sub>
<b>IUPAC Name</b>	5-(Aziridin-1-yl)-2,4-dinitrobenzamide
<b>InChI</b>	InChI=1S/C9H8N4O5/c10-9(14)5-3-7(11-1-2-11)8(13(17)18)4-6(5)12(15)16/h3-4H,1-2H2,(H2,10,14)
<b>InChI Key</b>	WOCXQMCLOTUMJV-UHFFFAOYSA-N
<b>Canonical SMILES</b>	C1CN1C2=C(C=C(C(=C2)C(=O)N)[N+](=O)[O-])[N+](=O)[O-]
<b>Isomeric SMILES</b>	CC#CCC(C)[C@@H](/C=C/[C@H]1[C@@H](C[C@H]2[C@@H]1C/C(=C/CCCC(=O)O)/C2)O)O
<b>Form</b>	Lyophilized powder
<b>Purity</b>	≥98%
<b>Impurities</b>	Free from inappropriate visible particulates, foreign matter, discoloration, or other defects.
<b>Solubility</b>	<i>In vitro</i> : DMSO: 49 mg/mL (194.3 mM); Water: insoluble; Ethanol: insoluble
<b>Identity</b>	Confirmed by NMR/HPLC/MS.
<b>Stability</b>	In its lyophilized form, the chemical remains stable for 36 months.
<b>Quality Level</b>	Research grade
<b>Applications</b>	CB1954 can be used for its ability to inhibit DNA synthesis and repair mechanisms through the formation of DNA cross-links.
<b>Storage</b>	Store at -20°C, and keep desiccated.



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