

## Product Information

### PR-104, Purity $\geq 98\%$

**Cat. No.:** X24-09-YM1261

**Size:** 5 mg; 10 mg; 25 mg; 50 mg

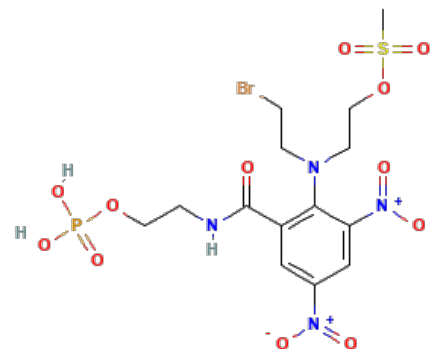
**CAS Number:** 851627-62-8

**Compound CID:** 11455973

**Synonym:** 851627-62-8; PR 104; PR104;

2-[N-(2-Bromoethyl)-2,4-dinitro-6-(2-phosphonooxyethylcarbamoyl)anilino]ethyl methanesulfonate

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



### Product Information

<b>Description</b>	PR-104 is a non-toxic, small-molecule, hypoxia-activated, 3,5-dinitrobenzamide nitrogen mustard pre-prodrug. The molecular weight of the compound is 579.27, and its molecular formula is $C_{14}H_{20}BrN_4O_{12}PS$ .
<b>Molecular Weight</b>	579.27
<b>Molecular Formula</b>	$C_{14}H_{20}BrN_4O_{12}PS$
<b>IUPAC Name</b>	2-[N-(2-Bromoethyl)-2,4-dinitro-6-(2-phosphonooxyethylcarbamoyl)anilino]ethyl methanesulfonate
<b>InChI</b>	InChI=1S/C14H20BrN4O12PS/c1-33(28,29)31-7-5-17(4-2-15)13-11(14(20)16-3-6-30-32(25,26)27)8-10(18(21)22)9-12(13)19(23)24/h8-9H,2-7H2,1H3,(H,16,20)(H2,25,26,27)
<b>InChI Key</b>	GZSOKPMDWVRVMG-UHFFFAOYSA-N
<b>Canonical SMILES</b>	<chem>CS(=O)(=O)OCCN(CCBrc1c(C=C(C=C1[N+](=O)[O-])[N+](=O)[O-])C(=O)NCCOP(=O)(O)O</chem>
<b>Isomeric SMILES</b>	<chem>C1[C@H]2[C@@H]([C@@H](S1)CCCC(=O)NN)NC(=O)N2</chem>
<b>Form</b>	Lyophilized powder
<b>Purity</b>	$\geq 98\%$
<b>Impurities</b>	Free from inappropriate visible particulates, foreign matter, discoloration, or other defects.
<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>	PR-104 can be studied extensively for its potential therapeutic applications in the treatment of oncology.
<b>Storage</b>	Store at $-20^{\circ}C$ , and keep desiccated.



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