

Product Information

Cytochrome P450 inhibitor, TH-302, Purity ≥98%

Cat. No.: X24-08-YM386

Size: 5 mg; 10 mg; 50 mg; 100 mg

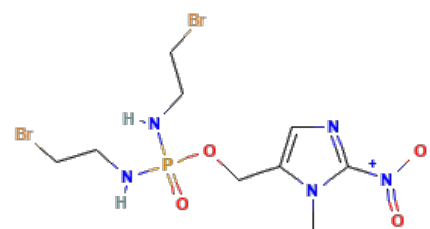
CAS Number: 918633-87-1

Compound CID: 11984561

Synonym: 918633-87-1; TH302; Evofosfamide;

2-Bromo-*N*

-(2-bromoethylamino)-[(3-methyl-2-nitroimidazol-4-yl)methoxy]phosphoryl]ethanamine



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

Product Information

Description	TH-302, soluble in DMSO, warmed water and ethanol, is an effective cell metabolism inhibitor, that has the ability to prevent the pathway of metabolism by inhibiting cytochrome P450.
Molecular Weight	449
Molecular Formula	C ₉ H ₁₆ Br ₂ N ₅ O ₄ P
IUPAC Name	2-Bromo- <i>N</i> -[(2-bromoethylamino)-[(3-methyl-2-nitroimidazol-4-yl)methoxy]phosphoryl]ethanamine
InChI	InChI=1S/C9H16Br2N5O4P/c1-15-8(6-12-9(15)16(17)18)7-20-21(19,13-4-2-10)14-5-3-11/h6H,2-5,7H2,1H3,(H2,13,14,19)
InChI Key	UWFYSQMTEOIJG-FDTZYFLXSA-N
Canonical SMILES	CC(=O)C1(CCC2C1(CCC3C2C=C(C4=CC(=O)C5CC5C34C)Cl)C)OC(=O)C
Isomeric SMILES	CC(=O)[C@]1(CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2C=C(C4=CC(=O)[C@@H]5C[C@@H]5[C@@]34C)Cl)C)OC(=O)C
Form	Lyophilized powder
Purity	≥98%
Titer	Free from inappropriate visible particulates, foreign matter, discoloration, or other defects
Solubility	<i>In vitro</i> : DMSO: 80 mg/mL (178.15 mM); Water (warmed): 9 mg/mL (20.03 mM); Ethanol: 80 mg/mL (178.15 mM); <i>In vivo</i> : 30% propylene glycol, 5% Tween 80, 65% D5W, 28 mg/mL
Stability	In its lyophilized form, the chemical remains stable for 36 months.
Quality Level	Research grade
Applications	TH-302 is a metabolism inhibitor that can be used for its ability to release cytotoxic agents in low-



oxygen environments typical of solid tumors.

Storage

Store at -20°C, and keep desiccated.
