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Typical Product Specifications & Properties

Fluoromethotrexate

CAS Number: : 95755-20-7

Specifications	Limits
Molecular weight	472.44
SMILES	<chem>n1c(c2nc(cnc2nc1N)CN(c1ccc(cc1)C(N[C@@H])(C[C@@H](C(=O)O)F)C(O)=O)=O)C)N</chem>
InChI	FPCVFWSJHMLPDB-UHFFFAOYSA-N
InChIKey	1S/C20H21FN8O5/c1-29(8-10-7-24-16-14(25-10)15(22)27-20(23)28-16)11-4-2-9(3-5-11)17(30)26-13(19(33)34)6-12(21)18(31)32/h2-5,7,12-13H,6,8H2,1H3,(H,26,30)(H,31,32)(H,33,34)(H4,22,23,24,27,28)



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