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Typical Product Specifications & Properties

(3,4-Dehydro-Pro3)-Tuftsia

CAS Number: : 91502-65-7

Specifications	Limits
Molecular weight	498.58
SMILES	<chem>C[C@H]([C@H](N)C(N[C@@H](CCCCN)C(=O)N1[C@@H](C=CC1)C(N[C@@H](CCCNC(N)=N)C(O)=O)=O)=O)O</chem>
InChI	OHGJMPDANPWMKQ-NNFXCFJSSA-N
InChIKey	1S/C21H38N8O6/c1-12(30)16(23)18(32)27-13(6-2-3-9-22)19(33)29-11-5-8-15(29)17(31)28-14(20(34)35)7-4-10-26-21(24)25/h5,8,12-16,30H,2-4,6-7,9-11,22-23H2,1H3,(H,27,32)(H,28,31)(H,34,35)(H4,24,25,26)/t12-,13?,14+,15+,16+/m1/s1



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