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Typical Product Specifications & Properties

Cyclo[L-Thr-[(3S,4S)-3-hydroxy-4-methyl-L-Pro]-[(4R,5R)-4,5-dihydroxy-N2-[(9Z,12Z)-1-oxo-9,12-octad

CAS Number: : 54651-05-7

Specifications	Limits
Molecular weight	1,074.27
SMILES	<chem>CCCCC\C=C/C\C=C/CCCCCCCC(=O)N[C@H]1C[C@@H](O)[C@@H](O)NC(=O)[C@@H]2[C@@H](O)[C@@H](C)CN2C(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]3C[C@@H](O)CN3C(=O)[C@@H](NC1=O)[C@@H](C)O)[C@H](O)[C@@H](O)c4ccc(O)cc4)[C@@H](C)O</chem>
InChI	FAUOJMHVEYMQQG-HVYQDZ ECSA-N
InChIKey	1S/C52H81N7O16/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-38(65)53-35-26-37(64)48(71)57-50(73)42-43(66)29(2)27-59(42)52(75)40(31(4)61)55-49(72)41(45(68)44(67)32-21-23-33(62)24-22-32)56-47(70)36-25-34(63)28-58(36)51(74)39(30(3)60)54-46(35)69/h9-10,



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