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Typical Product Specifications & Properties

Neoral

CAS Number: : 223528-56-1

Specifications	Limits
Molecular weight	1,202.62
SMILES	<chem>CC[C@H]1C(=O)N(CC(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N[C@@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N1)[C@@H]([C@H](C)C/C=C/C)O)C)C(C)C)C)CC(C)C)C)CC(C)C)C)C)CC(C</chem>
InChI	PMATZTZNYRCHOR-CGLBZJNRSA-N
InChIKey	1S/C62H111N11O12/c1-25-27-28-40(15)52(75)51-56(79)65-43(24)48(74)68(19)44(29-34(3)4)55(78)66-49(38(11)12)61(84)69(20)41(16)53(76)64-42(17)57(80)70(21)46(31-36(7)8)59(82)71(22)43(7)37(9)10)60(83)72(23)50(39(13)1
Melting Point	148-151 ° C
log P (octanol-water)	2.92
Atmospheric OH Rate Constant	3.46E-10 cm ³ /molecule-sec



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