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## Typical Product Specifications & Properties

# ALPHA-HEDERIN

CAS Number: : 27013-91-8

Specifications	Limits
Molecular weight	764.98
EINECS	248-166-5
SMILES	<chem>C1=2[C@@]([C@@]3([C@@H]([C@@]4(CC[C@@H]([C@@]([C@@H]4CC3)(CO)C)O[C@H]3[C@H](O[C@H]4[C@@H]([C@H](O)[C@H]([C@@H](O4)C)O)O)[C@@H](O)[C@H](CO3)O)C)CC2)C)(CC[C@@]2(C(=O)O)CCC(C[C@@H]12)(C)C)C</chem>
InChI	KEOITPILCOILGM-LLJOFIVSA-N
InChIKey	1S/C41H66O12/c1-21-28(44)30(46)31(47)33(51-21)53-32-29(45)24(43)19-50-34(32)52-27-11-12-37(4)25(38(27,5)20-42)10-13-40(7)26(37)9-8-22-23-18-36(2,3)14-16-41(23,35(48)49)17-15-39(22,40)6/h8,21,23-34,42-47H,9-20H2,1-7H3,(H,48,49)/t21-,23-,24-,25+,26+,27



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