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Typical Product Specifications & Properties

Carbenoxolone

CAS Number: : 5697-56-3

Specifications	Limits
Molecular weight	570.76
EINECS	227-174-2
SMILES	<chem>C1([C@H]2[C@@]([C@@]3(C([C@@H]4[C@@](CC[C@@](C4)(C(O)=O)C)(C)CC3)=C1)C)(CC[C@@H]1[C@@]2(CC[C@@H](C1(C)C)OC(CCC(O)=O)=O)C)C)=O</chem>
InChI	OBZHEBDUNPOCJG-WBXJDKIVSA-N
InChIKey	1S/C34H50O7/c1-29(2)23-10-13-34(7)27(32(23,5)12-11-24(29)41-26(38)9-8-25(36)37)22(35)18-20-21-19-31(4,28(39)40)15-14-30(21,3)16-17-33(20,34)6/h18,21,23-24,27H,8-17,19H2,1-7H3,(H,36,37)(H,39,40)/t21-,23-,24-,27+,30+,31-,32-,33+,34+/m0/s1
Melting Point	292.5 ° C
Atmospheric OH Rate Constant	1.08E-10 cm ³ /molecule-sec
log P (octanol-water)	7.060
Melting Point	291-294 °C
Density	1.20



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