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Typical Product Specifications & Properties

Cortolone-3-Glucuronide

CAS Number: : 95826-45-2

Specifications	Limits
Molecular weight	679.95
SMILES	<chem>C1(C(C(C(C(O1)OC1CCC2C(C1)(C1C(CC2)C2C(CC1=O)(C(CC2)(C(CO)O)O)C)C)O)O)C(=O)O.[Ba+2]</chem>
InChI	JFZNUBRLDQSHKU-UHFFFAOYSA-N
InChIKey	1S/C27H42O11.Ba/c1-25-9-13(37-24-21(33)19(31)20(32)22(38-24)23(34)35)5-3-12(25)4-6-14-15-7-8-27(36,17(30)11-28)26(15,2)10-16(29)18(14)25;/h12-15,17-22,24,28,30-33,36H,3-11H2,1-2H3,(H,34,35);/q:+2



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