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Typical Product Specifications & Properties

7-Ketodeoxycholic Acid

CAS Number: : 911-40-0

Specifications	Limits
Molecular weight	406.56
SMILES	<chem>C1[C@H](C[C@H]2CC([C@H]3[C@@H]4CC[C@H]([C@@H](CCC(=O)O)C)[C@@]4(C)[C@H](C[C@H]3[C@@]2(C1)C)O)=O)O</chem>
InChI	RHCPKKNRWFXMAT-RRWYKFPJSA-N
InChIKey	1S/C24H38O5/c1-13(4-7-21(28)29)16-5-6-17-22-18(12-20(27)24(16,17)3)23(2)9-8-15(25)10-14(23)11-19(22)26/h13-18,20,22,25,27H,4-12H2,1-3H3,(H,28,29)/t13-,14+,15-,16-,17+,18+,20+,22+,23+,24-/m1/s1



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