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Typical Product Specifications & Properties

Taurolithocholic Acid Sodium Salt

CAS Number: : 6042-32-6

Specifications	Limits
Molecular weight	505.69
SMILES	<chem>S(CCNC(CC[C@H]([C@@H]1[C@@]2([C@H]([C@@H]3CC[C@H]4[C@@]([C@@H]3CC2)(CC[C@H](O)C4)C)CC1)C)C)=O)(=O)(=O)[O-].[Na+]</chem>
InChI	YAERYJYXPRIDTO-XOGHUACDSA-M
InChIKey	1S/C26H45NO5S.Na/c1-17(4-9-24(29)27-14-15-33(30,31)32)21-7-8-22-20-6-5-18-16-19(28)10-12-25(18,2)23(20)11-13-26(21,22)3;/h17-23,28H,4-16H2,1-3H3,(H,27,29)(H,30,31,32);/q;+1/p-1/t17-,18-,19-,20+,21-,22+,23?,25+,26-;/m1./s1



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