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Typical Product Specifications & Properties

Taurodeoxycholic Acid Sodium Salt

CAS Number: : 1180-95-6

Specifications	Limits
Molecular weight	521.69
EINECS	214-652-0
SMILES	<chem>[Na+].C[C@H](CCC(=O)NCCS(=O)(=O)[O-])[C@H]1CC[C@H]2[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@]12C</chem>
InChI	YXHRQQJFKOHLAP-FVCKGWAHSA-M
InChIKey	1S/C26H45NO6S.Na/c1-16(4-9-24(30)27-12-13-34(31,32)33)20-7-8-21-19-6-5-17-14-18(28)10-11-25(17,2)22(19)15-23(29)26(20,21)3;/h16-23,28-29H,4-15H2,1-3H3,(H,27,30)(H,31,32,33);/q;+1/p-1/t16-,17-,18-,19+,20-,21+,22+,23+,25+,26-;/m1./s1
Water solubility	soluble
Storage Temperature	Freezer (-20°C)
Melting Point	168 °C (dec.)
Alpha	33 ° (c=3, water)
Solubility	H2O: 0.5 M at 20 °C, clear, colorless to faintly yellow



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415 Huguenot Street, New Rochelle, New York 10801

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