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## Typical Product Specifications & Properties

# Glycohyodeoxycholic acid

CAS Number: : 13042-33-6

Specifications	Limits
Molecular weight	449.63
SMILES	<chem>C1C[C@@]2([C@H]3CC[C@@]4([C@H](CC[C@@H]4[C@@H]3C[C@@H](O)[C@@H]2C[C@@H]1O)[C@H](C)CCC(=O)NCC(=O)O)C)C</chem>
InChI	SPOIYSFQOFYOFZ-BRDORRHWSA-N
InChIKey	1S/C26H43NO5/c1-15(4-7-23(30)27-14-24(31)32)18-5-6-19-17-13-22(29)21-12-16(28)8-10-26(21,3)20(17)9-11-25(18,19)2/h15-22,28-29H,4-14H2,1-3H3,(H,27,30)(H,31,32)/t15-,16-,17+,18-,19+,20+,21+,22+,25-,26-/m1/s1
Water solubility	28.2 mg/L
Henry's Law Constant	9.38E-17 atm-m <sup>3</sup> /mole
log P (octanol-water)	2.15
Atmospheric OH Rate Constant	6.42E-11 cm <sup>3</sup> /molecule-sec
Vapor Pressure	8.36E-18 mm Hg



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