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Typical Product Specifications & Properties

(2-hydroxyethyl)trimethylammonium (5 β)-3,7,12-trioxocholan-24-oate

CAS Number: : 4201-78-9

Specifications	Limits
Molecular weight	505.69
EINECS	224-106-3
SMILES	<chem>C[C@H](CCC(=O)[O-])[C@H]1CC[C@H]2[C@H]3[C@H](CC(=O)[C@]12C)[C@@]4(C)CCC(=O)C[C@H]4CC3=O.C[N+](C)(C)CCO</chem>
InChI	GJENZ XAFXDOTP-CAOXKPNISA-M
InChIKey	1S/C24H34O5.C5H14NO/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;1-6(2,3)4-5-7/h13-14,16-18,22H,4-12H2,1-3H3,(H,28,29);7H,4-5H2,1-3H3/q;+1/p-1/t13-,14+,16-,17+,18+,22+,23+,24-;/m1./s1



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