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Typical Product Specifications & Properties

Bucolome N-Glucuronide

CAS Number: : 98641-06-6

Specifications	Limits
SMILES	<chem>C1CCC([C@@H]2C(=O)[C@H]([C@H]3C[C@@H]([C@H]([C@@H]([C@H]3O)O)O)C([O-])=O)C([C@@H](CCCC)C2=O)=O)CC1.[Na+]</chem>
InChI	GSDWEDIBGZCBHU-AMIBHTEKSA-M
InChIKey	1S/C23H34O8.Na/c1-2-3-9-12-17(24)15(11-7-5-4-6-8-11)21(28)16(18(12)25)13-10-14(23(30)31)20(27)22(29)19(13)26;/h11-16,19-20,22,26-27,29H,2-10H2,1H3,(H,30,31);/q:+1/p-1/t12?,13?,14-,15?,16+,19-,20+,22+;/m0./s1



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