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## Typical Product Specifications & Properties

# Obacunon

CAS Number: : 751-03-1

Specifications	Limits
Molecular weight	454.52
SMILES	<chem>O1C(C=C[C@@]2([C@@H]3[C@@](C(C[C@@H]2C1(C)C)=O)([C@]12[C@H](C(O[C@H]([C@]2(C)CC3)c2cocc2)=O)O1)C)C)=O</chem>
InChI	MAYJEFRPIKEYBL-OASIGRBWSA-N
InChIKey	1S/C26H30O7/c1-22(2)16-12-17(27)25(5)15(23(16,3)9-7-18(28)32-22)6-10-24(4)19(14-8-11-30-13-14)31-21(29)20-26(24,25)33-20/h7-9,11,13,15-16,19-20H,6,10,12H2,1-5H3/t15-,16+,19+,20-,23-,24+,25+,26-/m1/s1



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