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Typical Product Specifications & Properties

Carubicin

CAS Number : 50935-04-1

Specifications	Limits
Molecular weight	513.49
SMILES	<chem>C[C@@H]1O[C@H](C[C@H](N)[C@@H]1O)O[C@H]2C[C@@](O)(Cc3c(O)c4C(=O)c5cccc(O)c5C(=O)c4c(O)c23)C(=O)C</chem>
InChI	XREUEWVEMYWFFA-CSKJXFQVSA-N
InChIKey	1S/C26H27NO10/c1-9-21(30)13(27)6-16(36-9)37-15-8-26(35,10(2)28)7-12-18(15)25(34)20-19(23(12)32)22(31)11-4-3-5-14(29)17(11)24(20)33/h3-5,9,13,15-16,21,29-30,32,34-35H,6-8,27H2,1-2H3/t9-,13-,15-,16-,21+,26-/m0/s1
Atmospheric OH Rate Constant	1.46E-10 cm ³ /molecule-sec
log P (octanol-water)	2.400



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