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Typical Product Specifications & Properties

Cefotiam Hexetil Hydrochloride

CAS Number: : 95789-30-3

Specifications	Limits
Molecular weight	768.77
SMILES	<chem>Cl.Cl.CC(OC(=O)OC1CCCCC1)OC(=O)C2=C(CSc3nnnn3CC1(NC(=O)Cc5csc(N)n5)C(=O)N24</chem>
InChI	FFSANQNELHESQJ-LWBICVDYSA-N
InChIKey	1S/C27H37N9O7S3.2ClH/c1-15(42-27(40)43-18-7-5-4-6-8-18)41-232-33-35(26)10-9-34(2)3)12-44-23-20(22(38)36(21)23)30-19(37)17;;/h14-15,18,20,23H,4-13H2,1-3H3,(H2,28,29)(H,30,37);2*1H/t1
Molecular weight	404.93
SMILES	<chem>C12=CC(=O)CC[C@@]1([C@@H]1[C@@H](C=C2Cl)[C@H]2[C@@](OC(=O)C)C(=O)C)(CC1)C</chem>
InChI	1S/C23H29ClO4/c1-13(25)23(28-14(2)26)10-7-18-16-12-20(24)121(19,3)17(16)6-9-22(18,23)4/h11-12,16-18H,5-10H2,1-4H3
InChIKey	QMBJSIBWORFWQT-UHFFFAOYSA-N
Atmospheric OH Rate Constant	7.04E-11 cm ³ /molecule-sec
Melting Point	213 ° C
log P (octanol-water)	3.950



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