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Typical Product Specifications & Properties

DAGOACETATESALT

CAS Number: : 100929-53-1

Specifications	Limits
Molecular weight	573.64
SMILES	<chem>c1cc(C[C@H](N)C(N[C@@H](C(=O)NCC(=O)N(C)[C@@H](Cc2ccccc2)C(=O)NCCO)C)=O)ccc1O.O.C(C)=O</chem>
InChI	XZZYKCKUDLGXJA-NJUGUJQKSA-N
InChIKey	1S/C26H35N5O6.C2H4O2/c1-17(30-25(36)21(27)14-19-8-10-20(33)11-9-19)24(35)29-16-23(34)31(2)22(26(37)28-12-13-32)15-18-6-4-3-5-7-18;1-2(3)4/h3-11,17,21-22,32-33H,12-16,27H2,1-2H3,(H,28,37)(H,29,35)(H,30,36);1H3,(H,3,4)/t17-,21+,22+;/m1./s1



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