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Typical Product Specifications & Properties

Argatroban

CAS Number: : 141396-28-3

Specifications	Limits
Molecular weight	526.66
SMILES	<chem>O.C[C@@H]1CCN([C@H](C1)C(=O)O)C(=O)[C@H](CCCNC(=N)N)NS(=O)(=O)c2cccc3CC(C)CNc23</chem>
InChI	AIEZTKLTLCMZIA-CZSXT PSTSA-N
InChIKey	1S/C23H36N6O5S.H2O/c1-14-8-10-29(18(12-14)22(31)32)21(30)17(6-4-9-26-23(24)25)28-35(33,34)19-7-3-5-16-11-15(2)13-27-20(16)19;/h3,5,7,14-15,17-18,27-28H,4,6,8-13H2,1-2H3,(H,31,32)(H4,24,25,26);1H2/t14-,15?,17+,18-;/m1./s1



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