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Typical Product Specifications & Properties

Vorapaxar sulfate

CAS Number: : 705260-08-8

Specifications	Limits
Molecular weight	590.66
SMILES	<chem>CCOC(=O)N[C@@H]1CC[C@@H]2[C@@H](C1)C[C@@H]3[C@@H]([C@@H](C)OC3=O)[C@H]2\C=C\C4CCC(CN4)C5CCCC(F)C5.OS(=O)(=O)O</chem>
InChI	NQRYCIGCIAWEIC-CKLVGUEFSA-N
InChIKey	1S/C29H33FN2O4.H2O4S/c1-3-35-29(34)32-23-10-11-24-20(14-23)15-26-27(17(2)36-28(26)33)25(24)12-9-22-8-7-19(16-31-22)18-5-4-6-21(30)13-18;1-5(2,3)4/h4-9,12-13,16-17,20,23-27H,3,10-11,14-15H2,1-2H3,(H,32,34);(H2,1,2,3,4)/b12-9+;/t17-,20+,23-,24-,25+,26-,



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