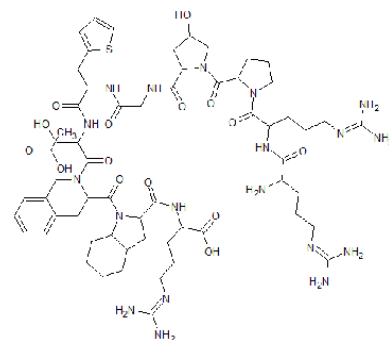


Icatibant Acetate

Catalog Number: EI-1194

CAS Number: 138614-30-9

Price: [Online Inquiry](#)



Catalog Number	Price
EI-1194	Online Inquiry

Product Information

Molecular Formula	C ₅₉ H ₈₉ N ₁₉ O ₁₃ S • XC ₂ H ₄ O ₂
Molecular Weight	1304.52
Purity	≥98%
SMILES	O=C(N1[C@](CCCC2)([H])[C@]2([H])C[C@H]1C(N[C@H](C(O)=O)CCCNC(N)=N)=O)[C@@H]3N(C([C@H](CO)NC([C@H](CC4=CC=CS4)NC(CNC([C@@H]5C[C@@H](O)CN5C([C@H]6N(C([C@@H](NC([C@H](N)CCCNC(N)=N)=O)CCCNC(N)=N)=O)CCC6)=O)=O)=O)=O)CC7=C(C=CC=C7)C3.O=C)O
InChi	InChI=1S/C59H89N19O13S.C2H4O2/c60-37(14-5-19-67-57(61)62)48(82)72-38(15-6-20-68-58(63)64)52(86)75-22-8-18-43(75)54(88)77-30-35(80)26-44(77)50(84)70-28-47(81)71-40(27-36-13-9-23-92-36)49(83)74-41(31-79)53(87)76-29-34-12-2-1-10-32(34)24-46(76)55(89)78-42-17-4-3-11-33(42)25-45(78)51(85)73-39(56(90)91)16-7-21-69-59(65)66;1-2(3)4/h1-2,9-10,12-13,23,33,35,37-46,79-80H,3-8,11,14-22,24-31,60H2,(H,70,84)(H,71,81)(H,72,82)(H,73,85)(H,74,83)(H,90,91)(H4,61,62,67)(H4,63,64,68)(H4,65,66,69);1H3,(H,3,4)/t33-,
InChi Key	HKMZRRZUEADSZDQ-DZJWSCHMSA-N
Alternate Name	HOE 140; D-arginyl-L-arginyl-L-prolyl-(4R)-4-hydroxy-L-prolyl-glycyl-3-(2-thienyl)-L-alanyl-L-seryl-(3R)-1,2,3,4-tetrahydro-3-isoquinolinecarbonyl-(2S,3aS,7aS)-octahydro-1H-indole-2-carbonyl-L-arginine, acetate
Appearance	White solid

Properties

Storage Conditions	-20°C
Shipping Conditions	Gel Pack

Solubility

>30 mg/ml DMSO