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Typical Product Specifications & Properties

Bosentan monohydrate

CAS Number: : 157212-55-0

Specifications	Limits
Molecular weight	569.63
SMILES	<chem>CC(C)(C)c1ccc(cc1)S(=O)(=O)Nc2c(c(nc(n2)c3nccccn3)OCCO)Oc4ccccc4OC.O</chem>
InChI	SXTRWVVIEPWAKM-UHFFFAOYSA-N
InChIKey	1S/C27H29N5O6S.H2O/c1-27(2,3)18-10-12-19(13-11-18)39(34,35)32-23-22(38-21-9-6-5-8-20(21)36-4)26(37-17-16-33)31-25(30-23)24-28-14-7-15-29-24;/h5-15,33H,16-17H2,1-4H3,(H,30,31,32);1H2



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