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Typical Product Specifications & Properties

Isometheptene Mucate, USP

CAS Number: : 7492-31-1

Specifications	Limits
Molecular weight	561.53
EINECS	231-315-3
SMILES	<chem>CC(CCC=C(C)C)NC.CC(CCC=C(C)C)NC.[C@@H]([C@@H]([C@H](C(=O)O)O)O)([C@@H](C(=O)O)O)O</chem>
InChI	WSXKZIDINJKWPM-IBGZLQDMSA-N
InChIKey	1S/2C9H19N.C6H10O8/c2*1-8(2)6-5-7-9(3)10-4;7-1(3(9)5(11)12)2(8)4(10)6(13)14/h2*6,9-10H,5,7H2,1-4H3;1-4,7-10H,(H,11,12)(H,13,14)/t;;1-,2+,3+,4-



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