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Typical Product Specifications & Properties

2,4-Hexadienoic acid, (E,E)-, compd. with [4S- (4a,4aa,5aa,6β,12aa)]-4- (dimethylamino)-1,4,4a,5,5a,6,

CAS Number: : 94237-34-0

Specifications	Limits
EINECS	304-130-1
SMILES	<chem>C/C=C/C=C/C(=O)O.C[C@@]1(c2ccccc(c2C(=O)C3=C([C@](C[C@@H]31)[C@@H](C(=C(C4=O)C(=O)N)O)N(C)C)O)O)</chem>
InChI	RTHISTRFAUBJKP-IQSJSTDGSA-N
InChIKey	1S/C22H24N2O8.C6H8O2/c1-21(31)8-5-4-6-11(25)12(8)16(26)10-15(24(2)3)17(27)14(20(23)30)19(29)22(10,32)18(13)28;1-2-6(7)8/h4-6,9-10,15,25,27-28,31-32H,7H2,1-3H3,(H2,23,30);2-5H,1(H,7,8)/b;3-2+,5-4+/t9-,10-,15-,21-,22-;/m0./s1



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