

Typical Product Specifications & Properties

4-{4-(Dimethylamino)-[(4''-Fluorophenyl)-1-Hydroxybutyl]-3-(Hydroxymethyl)}Benzonitrile

CAS Number: : 128173-53-5

Specifications	Limits
Molecular weight	1,071.18
SMILES	<chem>CN(C)CCC[C@](O)(c1ccc(F)cc1)c2ccc(cc2CO)C#N.CN(C)CCC[C@](O)(c3ccc(F)cc3)c4ccc(cc4CO)C#N.Cc5ccc(cc5)C(=O)O[C@@]([C@H](OC(=O)c6ccc(C)cc6)C(=O)O)C(=O)O</chem>
InChI	XADVDTANOZJZTP-XZWFXUMZSA-N
InChIKey	1S/2C20H23FN2O2.C20H18O8/c2*1-23(2)11-3-10-20(25,17-5-7-18(21)8-6-17)19-9-4-15(13-22)12-16(19)14-24;1-11-3-7-13(8-4-11)19(25)27-15(17(21)22)16(18(23)24)28-20(26)14-9-5-12(2)6-14/h2*4-9,12,24-25H,3,10-11,14H2,1-2H3;3-10,15-16H,1-2H3,(H,21,22)(H,23,