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Typical Product Specifications & Properties

1-deoxy-1-(methylamino)-D-glucitol 3-(acetylamino)-5-(acetlymethylamino)-2,4,6-triiodobenzoate

CAS Number: : 7241-11-4

Specifications	Limits
Molecular weight	823.14
SMILES	<chem>CC(=O)Nc1c(c(c(c(c1)N(C)C(=O)C)I)C(=O)O)I.CNC[C@@H]([C@H]([C@@H]([C@@H](CO)O)O)O)O</chem>
InChI	TXKOGNLDVKUFSI-WZTVWXICSA-N
InChIKey	1S/C12H11I3N2O4.C7H17NO5/c1-4(18)16-10-7(13)6(12(20)21)8(14)11(9(10)15)17(3)5(2)19;1-8-2-4(10)6(12)7(13)5(11)3-9/h1-3H3,(H,16,18)(H,20,21);4-13H,2-3H2,1H3/t;4-,5+,6+,7+/m.0/s1



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