



Formula: C₁₂H₂₁NO₉

MW: 323.3

Salt: H₂O

CAS: 50998-13-5

TNP NUMBER: TNP00576

MDL NUMBER: MFCD09788028

IUPAC: methyl 5-(acetylamino)-2,4-dihydroxy-6-(1,2,3-trihydroxypropyl)-2H-3,4,5,6-tetrahydropyran-2-carboxylate

Smiles: COC(C1(OC(C(C(O)C1)NC(=O)C)C(C(O)CO)O)O)=O

THERAPEUTIC CATEGORY: Widely distributed throughout the animal kingdom

ACCEPTORS: 9

DONORS: 6

ROTATION BONDS: 11

N+O: 10

Chiral Centers: 6

LogP: -4.79

LogS: -1.41

LIPINSKI: 3

Synonyms: N-ACETYLNEURAMINIC ACID METHYL ESTER;N-ACETYLNEURAMIC ACID METHYL ESTER;N-ACETYL-D-NEURAMINIC ACID METHYL ESTER;N-Acetyneuraminic;N-Acetyl-D-neuraminic acid methyl ester 97%

CAS:50998-13-5

MF:C12H21NO9

MW:323.3

EINECS:

Product Categories:Aromatic Esters;13C & 2H Sugars;Carbohydrates & Derivatives;Carbohydrates A to;Carbohydrates A-CBiochemicals and Reagents;Carbohydrates;Monosaccharide N-Acetylneuraminic acid methyl ester

Chemical Properties: mp 193.5-194.5 storage temp. -20C

CAS DataBase Reference: 50998-13-5(

CAS DataBase Reference:) Xi WGK Germany 3 Hazard Note Irritant N-Acetylneuraminic acid methyl ester

Usage And Synthesis:

Chemical Properties: White Crystalline Solid N-Acetylneuraminic acid methyl ester

