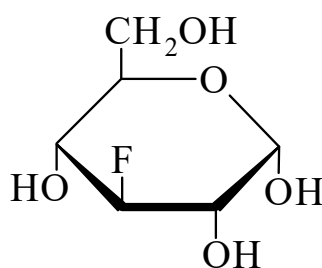




>>Entry Name: 3-Deoxy-3-fluoroglucose, 9Cl, 8Cl

Synonym(s): 3FG



α -D-Pyranose form

Molecular Formula: C₆H₁₁FO₅

Molecular Weight: 182.148

Accurate Mass: 182.059053

Percentage Composition: C 39.56%; H 6.09%; F 10.43%; O 43.92%

>>Variant: D-form

CAS Registry Number: 14049-03-7

Molecular Formula: C₆H₁₁FO₅

Molecular Weight: 182.148

Accurate Mass: 182.059053

Percentage Composition: C 39.56%; H 6.09%; F 10.43%; O 43.92%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 114-115°

Optical Rotation: [α]_D²⁵+66 (c, 0.7 in H₂O)

Other Data: Approx. equimolar amounts of α - and β -anomers

Aldrich: 32839-1

Fluka: 46865

Sigma: F7386

>>Derivative: 2,4-Dichlorophenylhydrazone

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 135°

>>Derivative: 6-Benzoyl

Synonym(s): 6-O-Benzoyl-3-deoxy-3-fluoro-D-glucose

CAS Registry Number: 56632-75-8

Molecular Formula: C₁₃H₁₅FO₆

Molecular Weight: 286.256

Accurate Mass: 286.085268

Percentage Composition: C 54.55%; H 5.28%; F 6.64%; O 33.54%

Optical Rotation: [α]_D²⁷+40 (c, 0.9 in EtOH)

>>Variant: α -D-Pyranose-form

CAS Registry Number: 31001-27-1

Molecular Formula: C₆H₁₁FO₅

Molecular Weight: 182.148

Accurate Mass: 182.059053

Percentage Composition: C 39.56%; H 6.09%; F 10.43%; O 43.92%

>>Derivative: 1,2,4,6-Tetra-Ac

Synonym(s): 1,2,4,6-Tetra-O-acetyl-3-deoxy-3-fluoro- α -D-glucopyranose

CAS Registry Number: 20409-32-9

Molecular Formula: C₁₄H₁₉FO₉

Molecular Weight: 350.297

Accurate Mass: 350.101313

Percentage Composition: C 48.00%; H 5.47%; F 5.42%; O 41.11%

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 109-111°

Optical Rotation: [α]_D²⁵+88 (c, 1.0 in CHCl₃)