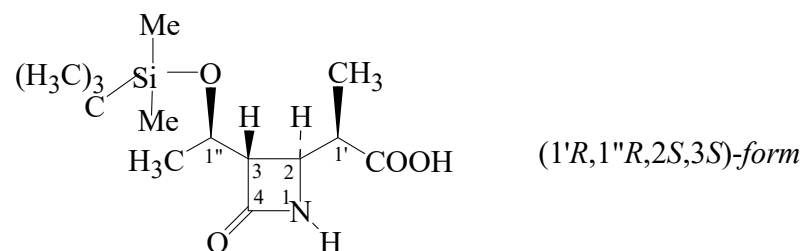




>>Entry Name: 3-[1-[(1,1-Dimethylethyl)dimethylsilyl]oxy]ethyl]- α -methyl-4-oxo-2-azetidineacetic acid, 9CI

Synonym(s): 3-[1-(*tert*-Butyldimethylsilyloxy)ethyl]-4-(1-carboxyethyl)-2-azetidinone



CAS Registry Number: 113033-46-8

Extra CAS Registry Numbers(s): 93711-85-4 120710-59-0 120710-60-3

Molecular Formula: C₁₄H₂₇NO₄Si

Molecular Weight: 301.457

Accurate Mass: 301.170936

Percentage Composition: C 55.78%; H 9.03%; N 4.65%; O 21.23%; Si 9.32%

Use/Importance: Intermed. to 1 β -methylcarbapenems

>>Variant: (1'*R*,1''*R*,2*S*,3*S*)-form

CAS Registry Number: 90776-58-2

Molecular Formula: C₁₄H₂₇NO₄Si

Molecular Weight: 301.457

Accurate Mass: 301.170936

Percentage Composition: C 55.78%; H 9.03%; N 4.65%; O 21.23%; Si 9.32%

Melting Point: Mp 152.5-153°

Optical Rotation: $[\alpha]_{\text{D}}^{20}$ -32.3 (c, 0.3 in MeOH)

>>Derivative: Me ester

CAS Registry Number: 87037-97-6

Molecular Formula: C₁₅H₂₉NO₄Si

Molecular Weight: 315.484

Accurate Mass: 315.186586

Percentage Composition: C 57.11%; H 9.26%; N 4.44%; O 20.29%; Si 8.90%

Melting Point: Mp 121-122°

Optical Rotation: $[\alpha]_{\text{D}}^{20}$ -27.8 (c, 0.39 in CHCl₃)

>>Derivative: Benzyl ester

CAS Registry Number: 96093-92-4

Molecular Formula: C₂₁H₃₃NO₄Si

Molecular Weight: 391.582

Accurate Mass: 391.217886

Percentage Composition: C 64.41%; H 8.49%; N 3.58%; O 16.34%; Si 7.17%

Physical Description: Cryst. (hexane)

Melting Point: Mp 69-70°

Optical Rotation: $[\alpha]_{\text{D}}^{20}$ -13.8 (c, 0.98 in CHCl₃)

>>Variant: (1'*S*,1''*R*,2*S*,3*S*)-form

CAS Registry Number: 97101-07-0

Molecular Formula: C₁₄H₂₇NO₄Si

Molecular Weight: 301.457

Accurate Mass: 301.170936

Percentage Composition: C 55.78%; H 9.03%; N 4.65%; O 21.23%; Si 9.32%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 189-190°

Optical Rotation: $[\alpha]_{\text{D}}^{25}$ -5 (c, 0.44 in MeOH)