



>>Entry Name: (Trimethylsilyl)acetic acid, 9Cl, 8Cl

CAS Registry Number: 2345-38-2

Me₃SiCH₂COOH

Molecular Formula: C₅H₁₂O₂Si

Molecular Weight: 132.234

Accurate Mass: 132.060657

Percentage Composition: C 45.42%; H 9.15%; O 24.20%; Si 21.24%

Source/Synthesis: Synth. from Me₃SiCH₂MgCl + CO₂

Use/Importance: Commercially available versatile synthon; dianion adds to ketones → RR'C=CHCOOH after elimination; also opens epoxides and substitutes alkyl bromides, iodides

Physical Description: Cryst.

Melting Point: Mp 40-42°

pKa Value: pK_{a1} 10 (MeOH) pK_{a1} 5.22 (H₂O)

Aldrich: 34161-4

Fluka: 92757

>>Derivative: Me ester

Synonym(s): Methyl trimethylsilylacetate

CAS Registry Number: 2916-76-9

Molecular Formula: C₆H₁₄O₂Si

Molecular Weight: 146.261

Accurate Mass: 146.076307

Percentage Composition: C 49.27%; H 9.65%; O 21.88%; Si 19.20%

Use/Importance: Commercially available; Li deriv. used in Peterson reaction

Physical Description: Liq.

Boiling Point: Bp₁₃ 38-39°

Refractive Index: n_D²⁰ 1.4140

Aldrich: 23496-6

Fluka: 92764

>>Derivative: Et ester

Synonym(s): Ethyl trimethylsilylacetate. ETSA

CAS Registry Number: 4071-88-9

Molecular Formula: C₇H₁₆O₂Si

Molecular Weight: 160.288

Accurate Mass: 160.091957

Percentage Composition: C 52.45%; H 10.06%; O 19.96%; Si 17.52%

Use/Importance: Commercially available silylating agent, also undergoes Reformatsky-type reactions; with catalytic Bu₄NF, silylates 1-alkynes, thiols; alcohols, ketones → silyl enol ethers. Li deriv. used in Peterson olefination of ketones; adds 1,4- to pyridinium salts; also couples with vinyl halides in presence of NiBr₂; adds to aldehydes, ketones to give alkylidenation

Physical Description: Moisture-sensitive liq.

Boiling Point: Bp 156-159°. Bp₄₀ 76-77°

Refractive Index: n_D²⁰ 1.4150

Aldrich: 20912-0

Fluka: 92756

Rare Chemicals Library: S3646-4

Sigma: E5880

>>Derivative: *tert*-Butyl ester

Synonym(s): *tert*-Butyl trimethylsilylacetate

CAS Registry Number: 41108-81-0

Molecular Formula: C₉H₂₀O₂Si

Molecular Weight: 188.341

Accurate Mass: 188.123257

Percentage Composition: C 57.40%; H 10.70%; O 16.99%; Si 14.91%

Use/Importance: Li deriv. adds to ketones; thermol. of product gives α,β-unsatd. esters (Peterson-type)

Physical Description: Liq.

Boiling Point: Bp₁₃ 67°