



>>Entry Name: 3-Phenyl-2*H*-azirine-2-carboxylic acid, 9Cl, 8Cl



Molecular Formula: C₉H₇NO₂

Molecular Weight: 161.16

Accurate Mass: 161.047679

Percentage Composition: C 67.08%; H 4.38%; N 8.69%; O 19.86%

>>Variant: (*S*)-form

Molecular Formula: C₉H₇NO₂

Molecular Weight: 161.16

Accurate Mass: 161.047679

Percentage Composition: C 67.08%; H 4.38%; N 8.69%; O 19.86%

>>Derivative: Me ester

CAS Registry Number: 163061-47-0

Molecular Formula: C₁₀H₉NO₂

Molecular Weight: 175.187

Accurate Mass: 175.063329

Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%

Physical Description: Yellow wax

Optical Rotation: [α]_D²⁰ +289.3 (c, 1.8 in CHCl₃)

>>Variant: ($\pm$)-form

Molecular Formula: C₉H₇NO₂

Molecular Weight: 161.16

Accurate Mass: 161.047679

Percentage Composition: C 67.08%; H 4.38%; N 8.69%; O 19.86%

>>Derivative: Me ester

CAS Registry Number: 18709-45-0

Molecular Formula: C₁₀H₉NO₂

Molecular Weight: 175.187

Accurate Mass: 175.063329

Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 45-45.5°

>>Derivative: Et ester

CAS Registry Number: 23893-63-2

Molecular Formula: C₁₁H₁₁NO₂

Molecular Weight: 189.213

Accurate Mass: 189.078979

Percentage Composition: C 69.83%; H 5.86%; N 7.40%; O 16.91%

Physical Description: Liq.

Boiling Point: Bp_{0.5} 92-95°

Refractive Index: n_D²³ 1.5370

>>Derivative: Amide

CAS Registry Number: 28883-94-5

Molecular Formula: C₉H₈N₂O

Molecular Weight: 160.175

Accurate Mass: 160.063663

Percentage Composition: C 67.49%; H 5.03%; N 17.49%; O 9.99%

Physical Description: Needles (C₆H₆)

Melting Point: Mp 187-189°

References: