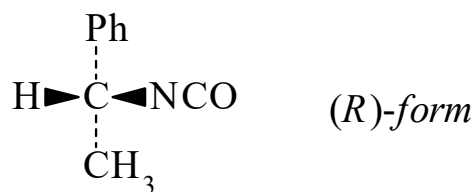




>>Entry Name: (1-Isocyanoethyl)benzene, 9CI

Synonym(s): 1-Phenylethyl isocyanate, 1-Isocyano-1-phenylethane



CAS Registry Number: 1837-73-6

Molecular Formula: $\text{C}_9\text{H}_9\text{NO}$

Molecular Weight: 147.176

Accurate Mass: 147.068414

Percentage Composition: C 73.45%; H 6.16%; N 9.52%; O 10.87%

>>Variant: (*R*)-form

CAS Registry Number: 33375-06-3

Molecular Formula: $\text{C}_9\text{H}_9\text{NO}$

Molecular Weight: 147.176

Accurate Mass: 147.068414

Percentage Composition: C 73.45%; H 6.16%; N 9.52%; O 10.87%

Use/Importance: Resolving agent for alcohols and amines

Aldrich: 42185-5

Fluka: 77973

Sigma: P1804

>>Variant: (*S*)-form

CAS Registry Number: 14649-03-7

Molecular Formula: $\text{C}_9\text{H}_9\text{NO}$

Molecular Weight: 147.176

Accurate Mass: 147.068414

Percentage Composition: C 73.45%; H 6.16%; N 9.52%; O 10.87%

Use/Importance: Resolving agent for alcohols and amines

Optical Rotation: $[\alpha]_{\text{D}} -17.4$ (c, 1.38 in C_6H_6)

Aldrich: 42186-3

Fluka: 77970

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

CAS Registry Number: 65451-96-9

Molecular Formula: $\text{C}_9\text{H}_9\text{NO}$

Molecular Weight: 147.176

Accurate Mass: 147.068414

Percentage Composition: C 73.45%; H 6.16%; N 9.52%; O 10.87%

Boiling Point: Bp_{12} 86-89°. $\text{Bp}_{0.4}$ 38°

Refractive Index: n_{D}^{20} 1.5151

References:

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