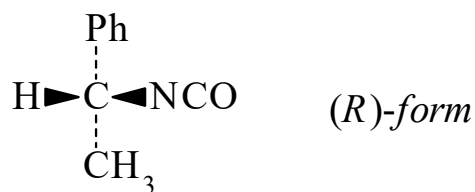




>>Entry Name: (1-Isocyanoethyl)benzene, 9CI

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



CAS Registry Number: 1837-73-6

Molecular Formula: C<sub>9</sub>H<sub>9</sub>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: C<sub>9</sub>H<sub>9</sub>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: C<sub>9</sub>H<sub>9</sub>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: [α]<sub>D</sub> −17.4 (c, 1.38 in C<sub>6</sub>H<sub>6</sub>)

Aldrich: 42186-3

Fluka: 77970

>>Variant: (±)-form

CAS Registry Number: 65451-96-9

Molecular Formula: C<sub>9</sub>H<sub>9</sub>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<sub>12</sub> 86-89°. Bp<sub>0.4</sub> 38°

Refractive Index: n<sub>D</sub><sup>20</sup> 1.5151

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