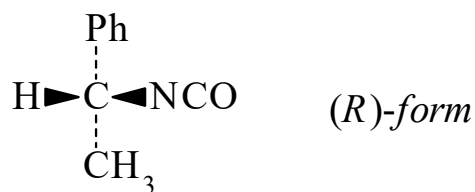




>>Entry Name: (1-Isocyanoethyl)benzene, 9CI

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:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1562B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 470C; 470D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1427A, (*ir*)

Cairns, T.L., *J.A.C.S.*, 1941, **63**, 871, (*synth*)

Hoover, F.W. *et al.*, *J.O.C.*, 1964, **29**, 163, (*synth*)

Freytag, W. *et al.*, *J. Chromatogr.*, 1969, **41**, 473, (*use*)

Hamberg, M., *Chem. Phys. Lipids*, 1971, **6**, 152, (*use*)

Maibaum, J., *J. Chromatogr.*, 1988, **436**, 269, (*use*)