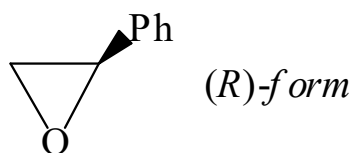




>>Entry Name: Phenyloxirane, 9CI

Synonym(s): (Epoxyethyl)benzene, 8CI. Styrene oxide. Phenylethylene oxide. Epoxystyrene



CAS Registry Number: 96-09-3

Extra CAS Registry Numbers(s): 67253-49-0

Molecular Formula: C_8H_8O

Molecular Weight: 120.151

Accurate Mass: 120.057515

Percentage Composition: C 79.97%; H 6.71%; O 13.32%

Use/Importance: Styrene metabolite

Hazard & Toxicity: Fl. p. 74° (oc), autoignition temp. 498°. Possible human carcinogen. Mod. human skin irritant and sensitiser. Eye irritant. LD₅₀ (rat, orl) 2000 mg/kg. LD₅₀ (rbt, skn) 1060 mg/kg. Exp. carcinogen. Exp. reprod. and teratogenic effects (by inhalation)

Aldrich: S500-6

Fluka: 77950

>>Variant: (R)-form

CAS Registry Number: 20780-53-4

Molecular Formula: C_8H_8O

Molecular Weight: 120.151

Accurate Mass: 120.057515

Percentage Composition: C 79.97%; H 6.71%; O 13.32%

Boiling Point: Bp₄ 57.5-58.5°

Optical Rotation: $[\alpha]_D^{29} +34.1$ (neat). $[\alpha]_D -22.5$ (CHCl₃)

Aldrich: 31029-8

Fluka: 78880

>>Variant: (S)-form

CAS Registry Number: 20780-54-5

Molecular Formula: C_8H_8O

Molecular Weight: 120.151

Accurate Mass: 120.057515

Percentage Composition: C 79.97%; H 6.71%; O 13.32%

Boiling Point: Bp 192-194°. Bp₁₀ 66-67°

Optical Rotation: $[\alpha]_D^{20} -33$ (neat). $[\alpha]_D^{25} -45.7$ (c, 1.25 in C₆H₆) (98% ee)

Density: d 1.051

Refractive Index: n_D^{20} 1.5350

Other: Kaneka H-5

>>Variant: (±)-form

Molecular Formula: C_8H_8O

Molecular Weight: 120.151

Accurate Mass: 120.057515

Percentage Composition: C 79.97%; H 6.71%; O 13.32%

Melting Point: Mp -37°

Boiling Point: Bp 194°. Bp₁₀ 75°. Bp₅ 65°

Solubility: Pract. insol. H₂O

Density: d_4^{16} 1.052

Refractive Index: n_D^{20} 1.5350

Other Data: Undergoes anionic and cationic polym.

References: