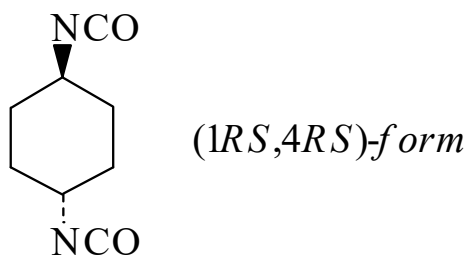




>>Entry Name: 1,4-Diisocyanatocyclohexane, 9CI

Synonym(s): 1,4-Cyclohexane diisocyanate



CAS Registry Number: 2556-36-7

Molecular Formula: C₈H₁₀N₂O₂

Molecular Weight: 166.179

Accurate Mass: 166.074228

Percentage Composition: C 57.82%; H 6.07%; N 16.86%; O 19.26%

>>Variant: (1*R*,4*R*)-form

Synonym(s): *trans*-form

CAS Registry Number: 7517-76-2

Molecular Formula: C₈H₁₀N₂O₂

Molecular Weight: 166.179

Accurate Mass: 166.074228

Percentage Composition: C 57.82%; H 6.07%; N 16.86%; O 19.26%

Use/Importance: Monomer for polyurethane elastomers

Physical Description: Liq.

Boiling Point: Bp₃₂ 145-146°. Bp₁₂ 122-124°

Aldrich: 26936-0

>>Derivative: Bis(methylurethane)

Physical Description: Cryst. (petrol)

Melting Point: Mp 63-64°

>>Variant: (1*R*,4*S*)-form

Synonym(s): *cis*-form

CAS Registry Number: 7517-77-3

Molecular Formula: C₈H₁₀N₂O₂

Molecular Weight: 166.179

Accurate Mass: 166.074228

Percentage Composition: C 57.82%; H 6.07%; N 16.86%; O 19.26%

Physical Description: Liq.

>>Derivative: Bis(methylurethane)

Melting Point: Mp 139-140°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1406A, (*nmr*)

Siefken, W., *Annalen*, 1960, **562**, 75, (*synth*)

U.K. Pat., 1968, 1 173 890; *CA*, **72**, 43115v, (*synth*)

Kozhevov, A.G. *et al.*, *CA*, 1971, **74**, 87475h, (*synth, struct*)

Wong, S.W. *et al.*, *Adv. Urethane Sci. Technol.*, 1981, **8**, 75, (*polymers*)

Encyclopaedia of Polymer Science and Engineering, Wiley-Interscience, New York, 2nd edn., 1988, **13**, 243, (*rev, polymers*)