



>>Entry Name: 4-Chloro-2-isocyanato-1-methylbenzene, 9CI

Synonym(s): 3-Chloro-6-methylphenyl isocyanate. 4-Chloro-2-isocyanatotoluene

CAS Registry Number: 40411-27-6

Structure by analogy with 1-Chloro-3-isocyanato-2-methylbenzene, [NPV57-I](#)

Molecular Formula: C₈H₆ClNO

Molecular Weight: 167.594

Accurate Mass: 167.013791

Percentage Composition: C 57.33%; H 3.61%; Cl 21.15%; N 8.36%; O 9.55%

Boiling Point: Bp₁₃ 102°

Refractive Index: n_D²⁰ 1.5562

Rare Chemicals Library: S55017-5

References:

Saunders, J.H. *et al.*, *Chem. Rev.*, 1948, **43**, 203, (*synth*)

Siefken, W., *Annalen*, 1949, **562**, 75, (*synth*)

Kaplan, M., *J. Chem. Eng. Data*, 1961, **6**, 272, (*synth*)

Klauke, E. *et al.*, *Synthesis*, 1978, 376, (*props*)