



>>Entry Name: 1-Chloro-4-isocyanato-2-(trifluoromethyl)benzene, 9Cl

Synonym(s): 4-Chloro- α,α,α -trifluoro-*m*-tolyl isocyanate, 8Cl. 4-Chloro-3-(trifluoromethyl)phenyl isocyanate

CAS Registry Number: 327-78-6

Structure by analogy with 1-Chloro-2-isocyanato-4-(trifluoromethyl)benzene, [KHC98-T](#)

Molecular Formula: C₈H₃ClF₃NO

Molecular Weight: 221.566

Accurate Mass: 220.985525

Percentage Composition: C 43.37%; H 1.36%; Cl 16.00%; F 25.72%; N 6.32%; O 7.22%

Melting Point: Mp 40-42° (27-27.5°)

Boiling Point: Bp₁₄ 86-90°

References:

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