



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

Synonym(s): 4-Chloro- α,α,α -trifluoro-*o*-tolyl isocyanate, 8Cl. 4-Chloro-2-(trifluoromethyl)phenyl isocyanate

CAS Registry Number: 16588-69-5

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

Molecular Formula: $\text{C}_8\text{H}_3\text{ClF}_3\text{NO}$

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%

Boiling Point: $\text{Bp}_{0.5}$ 64-64.5°

Density: d 1.47

Refractive Index: n_D^{20} 1.5010

References:

Commercially available and/or commonly cited compound for which no useful literature data is available, 1997