



>>Entry Name: **2-Isothiocyanto-2-methylpropane**, 9Cl

Synonym(s): *tert*-Butyl isothiocyanate, 8Cl. *tert*-Butyl mustard oil

CAS Registry Number: 590-42-1

(H₃C)₃CNCS

Molecular Formula: C₅H₉NS

Molecular Weight: 115.199

Accurate Mass: 115.045569

Percentage Composition: C 52.13%; H 7.87%; N 12.16%; S 27.84%

Melting Point: Mp 10.5-11.5°

Boiling Point: Bp 142°. Bp₁₀ 30.5-32°

Hazard & Toxicity: Irritant

Aldrich: 25185-2

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1411B, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 827C, (*ir*)

Kharasch, M.S. *et al.*, *J.A.C.S.*, 1937, **59**, 1580, (*synth*)

Schmidt, E. *et al.*, *Annalen*, 1950, **568**, 192, (*synth*)

Nair, G.V., *Indian J. Chem.*, 1966, **4**, 516, (*synth*)

Bäuerlein, E. *et al.*, *Annalen*, 1978, 675, (*synth*)

Kniezo, L. *et al.*, *Synth. Commun.*, 1990, **20**, 509, (*synth*)