



>>Entry Name: 1-Isothiocyanatohexane, 9CI

ENTRY UNDER REVIEW

Synonym(s): Hexyl isothiocyanate

CAS Registry Number: 4404-45-9

$\text{H}_3\text{C}(\text{CH}_2)_5\text{NCS}$

Molecular Formula: $\text{C}_7\text{H}_{13}\text{NS}$

Molecular Weight: 143.252

Accurate Mass: 143.076869

Percentage Composition: C 58.69%; H 9.15%; N 9.78%; S 22.38%

Biological Source: Isol. from radish (*Raphanus sativus*) and other crucifers

Physical Description: Liq.

Boiling Point: Bp 210°. Bp₂₇ 98°. Bp₁₅ 100°

Fluka: 53197

References:

Dyson, G.M. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1926, **45**, 421, (*synth*)

Svatek, E. *et al.*, *Acta Chem. Scand.*, 1959, **13**, 442, (*ir*, *uv*)

Kjaer, A. *et al.*, *Acta Chem. Scand.*, 1963, **17**, 2143, (*ms*)

Jensen, K.A. *et al.*, *Acta Chem. Scand.*, 1966, **20**, 2107, (*ms*)

Kjaer, A. *et al.*, *Agric. Biol. Chem.*, 1978, **42**, 1715, (*isol*)

Blotny, G., *Annalen*, 1982, 1927, (*synth*)

Yamamoto, T. *et al.*, *Org. Prep. Proced. Int.*, 1992, **24**, 346; 1994, **26**, 555, (*synth*, *ir*, *pmr*)