>>**Entry Name: 1-Isothiocyanatobutane,** 9CI
ENTRY UNDER REVIEW
Synonym(s): Butyl isothiocyanate, 8CI. Butyl mustard oil

CAS Registry Number: 592-82-5

$H_3C(CH_2)_3NCS$

Molecular Formula: C_5H_9NS
Molecular Weight: 115.199
Accurate Mass: 115.045569
Percentage Composition: C 52.13%; H 7.87%; N 12.16%; S 27.84%
Biological Source: Volatile constituent of cabbage and other crucifers arising from enzymic hydrolysis of Butyl glucosinolate LBB59-Y
Use/Importance: Shows fungicidal and insecticidal activity
Physical Description: Liq.
Boiling Point: Bp 167°. Bp_9 58-59°
Refractive Index: n_D^{20} 1.4980
Hazard & Toxicity: Irritant

Aldrich: 25379-0
Fluka: 20140

References:

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Jensen, K.A. *et al.*, *Acta Chem. Scand.*, 1966, **20**, 2107, *(ms)*
Kessler, H. *et al.*, *Chem. Ber.*, 1978, **111**, 2947, *(cmr)*
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