



>>Entry Name: **1-Isothiocyanato-2-methylpropane**, 9CI

Synonym(s): Isobutyl isothiocyanate, 8CI. Isobutyl mustard oil

CAS Registry Number: 591-82-2

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

Molecular Formula: $\text{C}_5\text{H}_9\text{NS}$

Molecular Weight: 115.199

Accurate Mass: 115.045569

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

Boiling Point: Bp₂₉ 72.5°

Density: d¹⁴ 0.964

Refractive Index: n_D¹⁴ 1.5005

Rare Chemicals Library: S52141-8

References:

Hodgkins, J.E., *J.O.C.*, 1956, **21**, 404, (*synth*)

Ohashi, M., *Acta Chem. Scand.*, 1963, **17**, 2143, (*synth, ms*)

Kjaer, A. *et al.*, *Phytochemistry*, 1978, **17**, 1285, (*isol*)

Olejniczak, B. *et al.*, *Synthesis*, 1989, 300, (*synth*)