



>>Entry Name: 2-Isothiocyanatobutane, 9CI

Synonym(s): *sec*-Butyl isothiocyanate. *sec*-Butyl mustard oil

CAS Registry Number: 4426-79-3

H3CCH2CH(NCS)CH3

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%

>>Variant: (+)-form

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%

Boiling Point: Bp 159°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +61.88$

>>Variant: (–)-form

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%

Boiling Point: Bp 159°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -61.8$

>>Variant: (±)-form

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%

Boiling Point: Bp 159.5°

References:

Hofmann, A.W., *Ber.*, 1874, **7**, 508, (*isol*)

Thomé, L.G., *Ber.*, 1903, **36**, 582, (*synth*)

Mumm, O. *et al.*, *Ber.*, 1940, **73**, 843, (*synth*)

Kim, S. *et al.*, *Tet. Lett.*, 1985, **26**, 1661, (*synth*)