



>>Entry Name: 1-Isothiocyanato-4-(methylsulfinyl)butane, 9CI

ENTRY UNDER REVIEW

Synonym(s): 4-(Methylsulfinyl)butyl isothiocyanate. **Sulforaphane**



CAS Registry Number: 4478-93-7

Molecular Formula: C₆H₁₁NOS₂

Molecular Weight: 177.291

Accurate Mass: 177.028204

Percentage Composition: C 40.65%; H 6.25%; N 7.90%; O 9.02%; S 36.17%

Use/Importance: Potent phase II enzymatic detoxification inhibitor, potential anticarcinogenic agent

Solubility: BERDY SOL: Sol. MeOH, Et₂O

Sigma: S0528

>>Variant: (*R*)-form

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Biological Source: Constit. of leaves of *Lepidum draba* and also present in *Brassica*, *Eruca* and *Iberis* spp.

Boiling Point: Bp_{0.03} 130-135°

Optical Rotation: [α]_D −79.3 (c, 1.2 in CHCl₃)

Solubility: BERDY SOL: Sol. MeOH, hexane; poorly sol. H₂O

>>Variant: (±)-form

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>>Derivative: Phenylthiourea deriv.

Melting Point: Mp 126-127°

References:

Schmid, H. *et al.*, *Helv. Chim. Acta*, 1948, **31**, 1497, (*synth, resoln*)

Procházka, Z., *Coll. Czech. Chem. Comm.*, 1959, **24**, 2429, (*synth*)

Balenovic, K. *et al.*, *Tetrahedron*, 1966, **22**, 2139, (*synth*)

Spencer, G.F. *et al.*, *J. Sci. Food Agric.*, 1980, **31**, 359, (*ms*)

Talalay, P. *et al.*, *Proc. Natl. Acad. Sci. U.S.A.*, 1992, **89**, 2399, (*pharmacol*)

Whitesell, J.K. *et al.*, *J.O.C.*, 1994, **59**, 597, (*synth*)

Chiang, W.C.K. *et al.*, *J. Agric. Food Chem.*, 1998, **46**, 1018-1021, (*anal, glc, ms*)