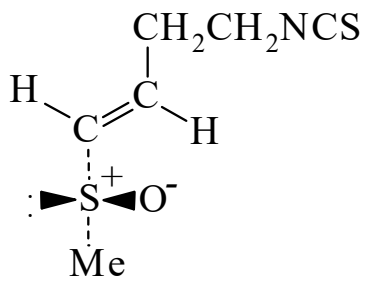




>>Entry Name: 4-Isothiocyanato-1-(methylsulfinyl)-1-butene, 9CI

ENTRY UNDER REVIEW

Synonym(s): Sulforaphene. Raphanin. Sulphoraphene



CAS Registry Number: 592-95-0

Molecular Formula: C₆H₉NOS₂

Molecular Weight: 175.275

Accurate Mass: 175.012554

Percentage Composition: C 41.12%; H 5.18%; N 7.99%; O 9.13%; S 36.59%

Use/Importance: Antibacterial, antifungal agent. Shows potential cancer protective properties

Calculated Log P Data: Log P 0.32 (uncertain value) (calc)

>>Variant: (R)-(E)-form

CAS Registry Number: 2404-46-8

Molecular Formula: C₆H₉NOS₂

Molecular Weight: 175.275

Accurate Mass: 175.012554

Percentage Composition: C 41.12%; H 5.18%; N 7.99%; O 9.13%; S 36.59%

bicornis

Boiling Point: Bp_{0.015} 125-130°

Optical Rotation: [α]_D -108 (c, 1.427 in CHCl₃)

Solubility: BERDY SOL: Sol. MeOH, CHCl₃, H₂O; fairly sol. Et₂O; poorly sol. hexane

UV: [neutral] λ_{max} 226 (ε 2951) (H₂O) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ivn) 10 mg/kg

References:

Schmid, H. *et al.*, *Helv. Chim. Acta*, 1948, **31**, 1017, (*synth*)

Cheung, K.K. *et al.*, *Chem. Comm.*, 1965, 100, (*synth*)

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

Kjaer, A. *et al.*, *Acta Chem. Scand., Ser. B*, 1974, **28**, 418, (*isol*)

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