



>>Entry Name: Benzyl glucosinolate

Synonym(s): 1-Thio-β-D-glucopyranose 1-[N-(sulfooxy)benzenethanimidate], 9Cl. **Glucotropaeolin.** Phenylmethyl glucosinolate

CAS Registry Number: 499-26-3

Related CAS Registry Numbers(s): 92761-40-5 117489-68-6

$\text{PhCH}_2\text{C}(\text{SGlc})=\text{NOSO}_3\text{H}$

Molecular Formula: $\text{C}_{14}\text{H}_{19}\text{NO}_9\text{S}_2$

Molecular Weight: 409.437

Accurate Mass: 409.050124

Percentage Composition: C 41.07%; H 4.68%; N 3.42%; O 35.17%; S 15.66%

Biological Source: Isol. from seeds of *Tropaeolum majus*, *Lepidium sativum* and other crucifers

Use/Importance: Possesses antibiotic props.

>>Derivative: K salt

CAS Registry Number: 5115-71-9

Physical Description: Amorph. powder

>>Derivative: Me_4N salt

Physical Description: Cryst.

Melting Point: Mp 188-189°

Optical Rotation: $[\alpha]_{\text{D}}^{28} -16.7$ (H_2O)

>>Derivative: Tetra-Ac

Physical Description: Cryst. +1 H_2O (EtOH aq.) (as K salt)

Melting Point: Mp 197-199 dec.° (K salt)

Optical Rotation: $[\alpha]_{\text{D}}^{25} -19$ (c, 0.5 in H_2O)

References:

Schultz, O.E. *et al.*, *Z. Naturforsch., B*, 1952, **7**, 500; 1953, **8**, 151, (*isol*)

Schultz, O.E. *et al.*, *Arch. Pharm. (Weinheim, Ger.)*, 1955, **288**, 525, (*isol*)

Ettlinger, M.G. *et al.*, *J.A.C.S.*, 1957, **79**, 1764, (*synth*)

Benn, M.H., *Can. J. Chem.*, 1963, **41**, 2836, (*synth*)

Underhill, E.W. *et al.*, *Biochem. Biophys. Res. Commun.*, 1964, **14**, 425, (*biosynth*)

Fenwick, G.R. *et al.*, *Biomed. Mass Spectrom.*, 1980, **7**, 410; 1981, **8**, 265, (*ms*)

Hanley, A.B. *et al.*, *J. Sci. Food Agric.*, 1983, **34**, 869, (*isol*)

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