



>>Entry Name: 4-(Methylthio)butyl glucosinolate

Synonym(s): 1-Thio- β -D-glucopyranose 1-[5-(methylthio)-N-(sulfooxy)pentanimidate], 9Cl. **Glucoerucin**

CAS Registry Number: 21973-56-8

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

Molecular Formula: $\text{C}_{12}\text{H}_{23}\text{NO}_9\text{S}_3$

Molecular Weight: 421.513

Accurate Mass: 421.053494

Percentage Composition: C 34.19%; H 5.50%; N 3.32%; O 34.16%; S 22.82%

>>Derivative: K salt

CAS Registry Number: 15592-37-7

Melting Point: Mp 153-154 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{26} -21.5$ (c, 0.55 in H_2O)

>>Derivative: Me_4N

Melting Point: Mp 159-161 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{26} -19.6$ (c, 0.6 in H_2O)

>>Derivative: Tetra-Ac

Melting Point: Mp 150-151 dec.° (as K salt)

Optical Rotation: $[\alpha]_{\text{D}}^{26} -14.9$ (c, 0.51 in H_2O)

>>Derivative: S-Oxide

Synonym(s): 4-(Methylsulfinyl)butyl glucosinolate. **Glucoraphanin**

CAS Registry Number: 21414-41-5

Molecular Formula: $\text{C}_{12}\text{H}_{23}\text{NO}_{10}\text{S}_3$

Molecular Weight: 437.512

Accurate Mass: 437.048409

Percentage Composition: C 32.94%; H 5.30%; N 3.20%; O 36.57%; S 21.99%

Biological Source: Isol. from radish (*Raphanus sativus*) and other crucifers

>>Derivative: S,S-Dioxide

References:

Schmidt, H. *et al.*, *Helv. Chim. Acta*, 1948, **31**, 1017, (*Glucoraphanin*)

Gmelin, R. *et al.*, *Acta Chem. Scand.*, 1968, **22**, 2875, (*Glucoerysolin*)

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

Cox, I.J. *et al.*, *Carbohydr. Res.*, 1984, **132**, 323, (*cmr*)