



>>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

MeSCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>C(SGlc)=NOSO<sub>3</sub>H

Molecular Formula: C<sub>12</sub>H<sub>23</sub>NO<sub>9</sub>S<sub>3</sub>

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:  $[\alpha]_D^{26} -21.5$  (c, 0.55 in H<sub>2</sub>O)

>>Derivative: Me<sub>4</sub>N

Melting Point: Mp 159-161 dec.°

Optical Rotation:  $[\alpha]_D^{26} -19.6$  (c, 0.6 in H<sub>2</sub>O)

>>Derivative: Tetra-Ac

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

Optical Rotation:  $[\alpha]_D^{26} -14.9$  (c, 0.51 in H<sub>2</sub>O)

>>Derivative: S-Oxide

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

CAS Registry Number: 21414-41-5

Molecular Formula: C<sub>12</sub>H<sub>23</sub>NO<sub>10</sub>S<sub>3</sub>

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*)