



>>Entry Name: Benzyl isothiocyanate

Synonym(s): (Isothiocyanatomethyl)benzene, 9Cl. Phenylmethyl isothiocyanate. Benzyl mustard oil. Tromocaps. Tromalyt active substance. Urogran

CAS Registry Number: 622-78-6

PhCH₂NCS

Molecular Formula: C₈H₇NS

Molecular Weight: 149.216

Accurate Mass: 149.029919

Percentage Composition: C 64.40%; H 4.73%; N 9.39%; S 21.49%

Biological Source: Isol. from *Tropaeolum majus* and *Lepidium sativum* and in other plants esp. in the Cruciferae. Formed from 3-Hydroxybenzyl glucosinolate [LBB09-J](#)

Use/Importance: Antineoplastic agent. Shows bactericidal, antiviral and fungicidal props. Inhibits tumourigenesis in animal models

Physical Description: Pale yellow oil or orange-red cryst.

Melting Point: Mp 41°

Boiling Point: Bp 243°. Bp₁₂ 125-126°

Calculated Log P Data: Log P 3.2 (calc)

Hazard & Toxicity: Severe irritant. LD₅₀ (mus, scu) 150 mg/kg ; BERDY HAZD : LD₅₀ (mus, scu) 150 mg/kg

Aldrich: 25249-2

Fluka: 13505

Rare Chemicals Library: S64549-4

References:

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