



>>Entry Name: 2-Propenylthiourea, 9CI

Synonym(s): Allylthiourea, INN. Allylthiocarbamide. Aminosin‡. Rhodallin. Rodalina. Thiosinamine. Tiosinamine. *N,N*-Diethyl-*N'*-2-propenylthiourea

CAS Registry Number: 109-57-9

$\text{H}_2\text{C}=\text{CHCH}_2\text{NHCSNH}_2$

Molecular Formula: $\text{C}_4\text{H}_8\text{N}_2\text{S}$

Molecular Weight: 116.187

Accurate Mass: 116.040818

Percentage Composition: C 41.35%; H 6.94%; N 24.11%; S 27.60%

Use/Importance: Used to minimise scar tissue

Physical Description: Monoclinic or rhombic prisms

Melting Point: Mp 78°. Mp 55°

Solubility: Sol. H_2O , EtOH, spar. sol. Et_2O , insol. C_6H_6

Calculated Log P Data: Log P -0.12 (calc)

Hazard & Toxicity: Powerful allergen. LD₅₀ (rat, ori) 200 mg/kg

Aldrich: 10880-4

Fluka: 6064

Sigma: T9162

>>Derivative: *N,N*-Di-Et

Synonym(s): *N,N*-Diethyl-*N'*-2-propenylthiourea, 9CI

CAS Registry Number: 21645-26-1

Molecular Formula: $\text{C}_8\text{H}_{16}\text{N}_2\text{S}$

Molecular Weight: 172.294

Accurate Mass: 172.103418

Percentage Composition: C 55.77%; H 9.36%; N 16.26%; S 18.61%

Physical Description: Prisms (EtOH)

Melting Point: Mp 55°

Other: PB: D19700

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 828D, (ir)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1337C, (nmr)

Gebhardt, W., *Ber.*, 1884, **17**, 3038, (*N,N*-di-Et)

Gadamer, J., *J.C.S.*, 1896, **70**, 414

Kofler, A., *Arch. Pharm. (Weinheim, Ger.)*, 1948, **281**, 8

Neville, R.G. *et al.*, *Can. J. Chem.*, 1963, **41**, 2123

Dragonette, K.S. *et al.*, *Acta Cryst.*, 1965, **19**, 973, (cryst struct)

Wolfgang, W. *et al.*, *Annalen*, 1971, **743**, 167, (ir)

Popiel, I. *et al.*, *Trans. R. Soc. Trop. Med. Hyg.*, 1981, **75**, 287, (props)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, AGT500