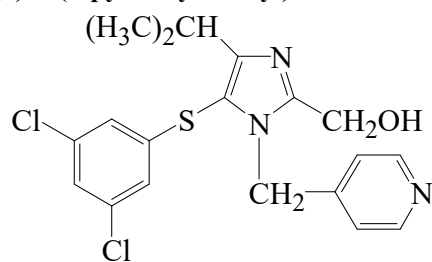




>>Entry Name: 5-[(3,5-Dichlorophenyl)thio]-4-(1-methylethyl)-1-(4-pyridinylmethyl)-1*H*-imidazole-2-methanol, 9Cl



CAS Registry Number: 178981-89-0

Molecular Formula: C₁₉H₁₉Cl₂N₃OS

Molecular Weight: 408.35

Accurate Mass: 407.062586

Percentage Composition: C 55.89%; H 4.69%; Cl 17.36%; N 10.29%; O 3.92%; S 7.85%

Melting Point: Mp 137-139°

>>**Derivative:** Hydrochloride (1:2)

Melting Point: Mp 223-235 dec.°

>>**Derivative:** Carbamoyl

Synonym(s): Capravirine, INN. AG 1549. S 1153

CAS Registry Number: 178979-85-6

Molecular Formula: C₂₀H₂₀Cl₂N₄O₂S

Molecular Weight: 451.375

Accurate Mass: 450.0684

Percentage Composition: C 53.22%; H 4.47%; Cl 15.71%; N 12.41%; O 7.09%; S 7.10%

Biological Use/Importance: HIV-1 reverse transcriptase inhibitor. Anti-HIV agent

Melting Point: Mp 88 dec.°

>>**Derivative:** Carbamoyl, hydrochloride (1:2)

Melting Point: Mp 214-222 dec.°

References:

Chinese Pat., 1994, *Shanghai Pharmaceutic Industry*, 1 096 514; *CA*, **124**, 87042r, (*synth, pharmacol*)

Eur. Pat., 1997, *Shionogi*, 786 455; *CA*, **125**, 114616k, (*synth, pharmacol*)

Fujiwara, T. *et al.*, *Antimicrob. Agents Chemother.*, 1998, **42**, 1340-1345, (*activity*)

Ohkawa, T. *et al.*, *Xenobiotica*, 1998, **28**, 877-886, (*metab*)

Ren, J. *et al.*, *J. Biol. Chem.*, 2000, **275**, 14316-14320, (*cryst struct, complex*)