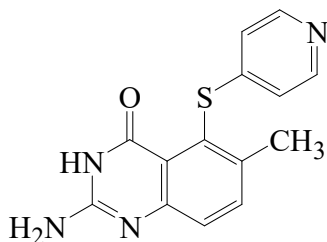




>>Entry Name: Nolatrexed, INN

Synonym(s): 2-Amino-6-methyl-5-(4-pyridinylthio)-4(1H)-quinazolinone, 9Cl. Thymitaq



CAS Registry Number: 147149-76-6

Related CAS Registry Numbers(s): 152946-64-0 181360-02-1

Molecular Formula: C₁₄H₁₂N₄OS

Molecular Weight: 284.341

Accurate Mass: 284.073181

Percentage Composition: C 59.14%; H 4.25%; N 19.70%; O 5.63%; S 11.28%

Biological Use/Importance: Thymidylate synthase inhibitor. Antineoplastic agent

Physical Description: Tan solid

Melting Point: Mp 301-302°

Calculated Log P Data: Log P 1.83 (calc)

>>Derivative: Hydrochloride (1:2)

Synonym(s): AG 337

CAS Registry Number: 152946-68-4

Physical Description: Cryst.

Melting Point: Mp 312° (dec.) (anhyd.)

Other Data: Exists as dihydrate

References:

- Webber, S.E. *et al.*, *J. Med. Chem.*, 1993, **36**, 733-746, (*synth, pharmacol, ir, pmr*)
Pat. Coop. Treaty (WIPO), 1993, *Agouron*, 93 20 055; *CA*, **120**, 164214v, (*synth, pharmacol*)
Rhee, M.S. *et al.*, *Cell. Pharmacol.*, 1995, **2**, 97-101, (*pharmacol*)
Webber, S. *et al.*, *Cancer Chemother. Pharmacol.*, 1996, **37**, 509-517, (*pharmacol*)
Dash, A.K. *et al.*, *J. Pharm. Sci.*, 1996, **85**, 1123-1127, (*struct*)