



>>Derivative: 9-Octadecenoyl (*E*-)

Synonym(s): 9-[2'-(9"-Octadecenoyloxy)ethoxymethyl]guanine. **Acyclovir elaidate**. P 4010

CAS Registry Number: 151090-37-8

Extra CAS Registry Numbers(s): 151090-36-7

Molecular Formula: C₂₆H₄₃N₅O₄

Molecular Weight: 489.657

Accurate Mass: 489.331505

Percentage Composition: C 63.78%; H 8.85%; N 14.30%; O 13.07%

Biological Use/Importance: Antiviral agent. Shows greater activity than parent compd.

>>Derivative: L-Valine ester

Synonym(s): **Valaciclovir**, BAN, INN. Valtrex. Zelitrex

CAS Registry Number: 124832-26-4

Molecular Formula: C₁₃H₂₀N₆O₄

Molecular Weight: 324.339

Accurate Mass: 324.154604

Percentage Composition: C 48.14%; H 6.22%; N 25.91%; O 19.73%

Biological Use/Importance: Antiviral agent; active against herpes

Physical Description: Cryst. (EtOH aq.)

Development Status: Approved for pharmaceutical use 1995

Calculated Log P Data: Log P -1.09 (calc)

>>Derivative: L-Valine ester; hydrochloride

Synonym(s): **Valacyclovir hydrochloride**, USAN. Valtrex

CAS Registry Number: 124832-27-5

Physical Description: Powder + 1H₂O (EtOH aq.)

Melting Point: Mp 150° (monohydrate)

Other Data: Dec. at 195°

References:

- Ger. Pat.*, 1976, 2 539 963; *CA*, **84**, 180300p, (*synth*)
Elion, G.B. *et al.*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 5716, (*pharmacol*)
Fiddian, A.P., *Appl. Virol.*, 1984, 103, (*rev, pharmacol*)
Birnbaum, G.I. *et al.*, *Can. J. Chem.*, 1984, **62**, 2646, (*cryst struct*)
Eur. Pat., 1984, *Wellcome*, 108 285; *CA*, **101**, 192401e, (*Desciclovir, synth, pharmacol*)
Krenitsky, T.A. *et al.*, *Proc. Natl. Acad. Sci. U.S.A.*, 1984, **81**, 3209-3213, (*synth, pharmacol*)
Krasny, H.C. *et al.*, *Biochem. Pharmacol.*, 1986, **35**, 4339, (*metab*)
Rees, P.J. *et al.*, *J. Antimicrob. Chemother.*, 1986, **18**, 215-222, (*pharmacokinet*)
Kelley, J.L. *et al.*, *J. Het. Chem.*, 1986, **23**, 271, (*synth*)
Chu, C.K. *et al.*, *J. Het. Chem.*, 1986, **23**, 289, (*rev*)
Radl, S. *et al.*, *Cesk. Farm.*, 1987, **36**, 58, (*synth*)
Petty, B.G. *et al.*, *Antimicrob. Agents Chemother.*, 1987, **31**, 1317-1322, (*pharmacokinet*)
Matsumoto, H. *et al.*, *Chem. Pharm. Bull.*, 1988, **36**, 1153, (*synth*)
Arndt, K.A. *et al.*, *J. Am. Acad. Dermatol.*, 1988, **18**, 188, (*adverse effects*)
Eur. Pat., 1989, *Wellcome*, 308 065; *CA*, **112**, 112048j, (*Valaciclovir*)
Stimac, A. *et al.*, *Synthesis*, 1990, 461-464, (*synth*)
Reardon, J.E. *et al.*, *Adv. Pharmacol.*, 1991, **22**, 1, (*rev*)
Alhede, B. *et al.*, *J.O.C.*, 1991, **56**, 2139, (*synth, cmr*)
De Miranda, P. *et al.*, *Antiviral Chem. Chemother.*, 1992, **3**, 1, (*metab, rev*)
Beauchamp, L.M. *et al.*, *Antiviral Chem. Chemother.*, 1992, **3**, 157, (*Valaciclovir*)
U.K. Pat., 1993, *Norsk Hydro A/S*, 2 260 319; *CA*, **119**, 271633g, (*acyclovir elaidate*)
De Miranda, P. *et al.*, *Drug Metab. Dispos.*, 1994, **22**, 55, (*Valaciclovir*)
Wagstaff, A.J. *et al.*, *Drugs*, 1994, **47**, 153, (*rev*)
Buck, I.M. *et al.*, *Tetrahedron*, 1994, **50**, 9195-9206, (*synth*)
Shinkai, I. *et al.*, *Bioorg. Med. Chem.*, 1996, **4**, 1, (*rev, Valaciclovir*)
Jennings, R. *et al.*, *Antimicrob. Agents Chemother.*, 1999, **43**, 53-61, (*acyclovir elaidate*)
Plass, M. *et al.*, *J.C.S. Perkin 2*, 1999, 2641-2646, (*uv, pmr, ir, Raman*)
Martindale, The Extra Pharmacopoeia, 32nd edn., *Pharmaceutical Press*, 1999, 602; 628
Ormrod, D. *et al.*, *Drugs*, 2000, **59**, 839-863; 1317-1359
Gao, H. *et al.*, *Synthesis*, 2000, 329-351, (*rev*)
Gao, H. *et al.*, *Synth. Commun.*, 2001, **31**, 1399-1419, (*synth*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., *Van Nostrand Reinhold*, 1992, AEC700; AEC725