Merck 13

Monograph Number: 3553
Title: Eflornithine
CAS Registry Number: 67037-37-0
CAS Name: 2-(Difluoromethyl)-DL-ornithine
Additional Names: α-difluoromethylornithine; DFMO
Manufacturers' Codes: RMI-71782
Molecular Formula: $C_6H_{12}F_2N_2O_2$
Molecular Weight: 182.17.
Percent Composition: C 39.56%, H 6.64%, F 20.86%, N 15.38%, O 17.57%

Literature References: Irreversible inhibitor of ornithine decarboxylase.
Prepn: B. W. Metcalf *et al., J. Am. Chem. Soc.* **100,** 2551 (1978);
P. Bey *et al., J. Org. Chem.* **44,** 2732 (1979).
Antiproliferative effects on cultured tumor cells: P. S. Mamont *et al., Biochem. Biophys. Res. Commun.* **81,** 58 (1978);
on Ehrlich ascites cells in rats: L. Alhonen-Hongisto *et al., Acta Chem. Scand.* **B33,** 559 (1979).
Inhibition of polyamine biosynthesis: E. Hölttä *et al., Biochem. J.* **178,** 109 (1979).
Antitrypanosomal activity in mice: C. J. Bacchi *et al., Science* **210,** 332 (1980).
Pharmacokinetics in humans: K. D. Haegele *et al., Clin. Pharmacol. Ther.* **30,** 210 (1981).
Clinical evaluations in *Pneumocystis carinii* pneumonia: J. A. Golden *et al., West. J. Med.* **141,** 613 (1984);
in trypanosomiasis: S. Van Nieuwenhove *et al., Trans. Royal Soc. Trop. Med. Hyg.* **79,** 692 (1985);
in cancer chemotherapy: M. D. Abeloff *et al., Cancer Treat. Rep.* **70,** 843 (1986);
V. A. Levin *et al., ibid.* **71,** 459 (1987).

Derivative Type: Hydrochloride monohydrate
CAS Registry Number: 96020-91-6
Trademarks: Ornidyl (HMR)
Molecular Formula: $C_6H_{12}F_2N_2O_2.HCl.H_2O$
Molecular Weight: 236.65.
Percent Composition: C 30.45%, H 6.39%, F 16.06%, N 11.84%, O 20.28%, Cl 14.98%
Properties: Crystals from ethanol/water, mp 183°.
Melting point: mp 183°

Therap-Cat: Antineoplastic; antipneumocystic; antiprotozoal (Trypanosoma).

Combined Chemical Dictionary
Synonym(s): 2-(Difluoromethyl)ornithine, 9CI . 2,5-Diamino-2-(difluoromethyl)pentanoic acid. Ornidyl. MDL 71782. RMI 71782. DFMO
Chapman and Hall Number: BDR18-V
CAS Registry Number: 70052-12-9
Type of Compound Code(s): XA2330 XA1950 XA2100
Molecular Formula: C 6 H 12 F 2 N 2 O 2
Molecular Weight: 182.17 **Accurate Mass**: 182.086684
Percentage Composition: C 39.56%; H 6.64%; F 20.86%; N 15.38%; O 17.57%

Use/Importance:
Antiprotozoal agent (ornithine decarboxylase inhibitor).
Used in the treatment of trypanosomiasis and Pneumocystis pneumonia.
Also shows some antineoplastic activity.
Also prevents increase in blood pressure in animal models of hypertension
Calculated Log P Data: Log P minus3 (uncertain value) (calc)
Hazard and Toxicity: Adverse gastrointestinal and haemopoietic effects reported. Exp. reprod. and teratogenic effects
RTECS Accession Number: RM2981700

Rare Chemicals Library: S1449-5

Variant: (+)-form
Chapman and Hall Number: BDR19-W
CAS Registry Number: 103957-16-0
Molecular Formula: C 6 H 12 F 2 N 2 O 2
Molecular Weight: 182.17 **Accurate Mass**: 182.086684
Percentage Composition: C 39.56%; H 6.64%; F 20.86%; N 15.38%; O 17.57%
Derivative: Hydrochloride
Chapman and Hall Number: BDR20-Q
CAS Registry Number: 70050-55-4
Physical Description: Cryst. (EtOH aq.)
Melting Point: Mp 240degrees
Optical Rotation: [alpha] D +7 (c, 0.48 in MeOH)

Variant: (minus)-form
Chapman and Hall Number: BDR21-R
CAS Registry Number: 66640-93-5
Molecular Formula: C 6 H 12 F 2 N 2 O 2
Molecular Weight: 182.17 **Accurate Mass**: 182.086684
Percentage Composition: C 39.56%; H 6.64%; F 20.86%; N 15.38%; O 17.57%
Derivative: Hydrochloride
Chapman and Hall Number: BDR22-S
CAS Registry Number: 69955-42-6
Physical Description: Cryst. (EtOH aq.)
Melting Point: Mp 244degrees
Optical Rotation: [alpha] D minus10 (c, 0.7 in MeOH)

Variant: (plus or minus)-form
Chapman and Hall Number: BDR23-T
CAS Registry Number: 67037-37-0
Molecular Formula: C 6 H 12 F 2 N 2 O 2
Molecular Weight: 182.17 **Accurate Mass**: 182.086684
Percentage Composition: C 39.56%; H 6.64%; F 20.86%; N 15.38%; O 17.57%
Derivative: Hydrochloride
Synonym(s): Eflornithine hydrochloride, USAN
Chapman and Hall Number: BDR24-U
CAS Registry Number: 68278-23-9
Physical Description: Cryst. + 1H 2 O (EtOH aq.)
Melting Point: Mp 183degrees
RTECS Accession Number: RM2981900

References:

Bey, P. et al. , J.O.C. , 1979, 44 , 2732, (synth)
McCann, P.P. et al. , Adv. Polyamine Res. , 1981, 3 , 97, (rev, pharmacol)
Janne, J. et al. , Med. Biol. , 1981, 59 , 448, (rev, pharmacol)
Fozard, J.R. et al. , Trends Pharmacol. Sci. , 1982, 3 , 107, (rev, pharmacol)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press , 1993, 513
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