



CAS Registry Number: 709-55-7

Molecular Formula: C₁₀H₁₅NO₂

Molecular Weight: 181.234

Accurate Mass: 181.110279

Percentage Composition: C 66.27%; H 8.34%; N 7.73%; O 17.66%

Use/Importance: Analeptic, sympathomimetic agent

Melting Point: Mp 147-148°

Calculated Log P Data: Log P 0.44 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 114 mg/kg. Exp. reprod. and teratogenic effects

>>**Derivative:** *N*-Et; hydrochloride

Synonym(s): Etilefrine hydrochloride, JAN. Circupon. Apocretin. Eftortil. Palsamin. Kertasin. Pressoton. Effoless. Sanlephrin. M-I-36

CAS Registry Number: 943-17-9

Melting Point: Mp 121°

Rare Chemicals Library: S44726-9

>>**Derivative:** *N*-Et, *O*³-(2,2-dimethylpropanoyl)

Synonym(s): Etilefrine pivalate, INN. K 30052

CAS Registry Number: 85750-39-6

Molecular Formula: C₁₅H₂₃NO₃

Molecular Weight: 265.352

Accurate Mass: 265.167794

Percentage Composition: C 67.90%; H 8.74%; N 5.28%; O 18.09%

Use/Importance: Sympathomimetic

>>**Derivative:** *N*-Et, *O*³-(2,2-dimethylpropanoyl); hydrochloride

CAS Registry Number: 42145-91-5

Physical Description: Cryst. (2-propanol)

Melting Point: Mp 209.4°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 604A; 604B, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1285D; 1286A, (*ir*)
Bretschneider, H. *et al.*, *Monatsh. Chem.*, 1950, **81**, 31, (*resoln*)
Hartman, W.J. *et al.*, *J.A.C.S.*, 1955, **77**, 816, (*biosynth*)
D'Amico *et al.*, *Chim. Ind. (Milan)*, 1956, **38**, 93, (*synth, resoln*)
Chatterjee, A. *et al.*, *J.C.S.*, 1961, 4576, (*synth*)
Thies, H. *et al.*, *Arch. Pharm. (Weinheim, Ger.)*, 1962, **295**, 194, (*uv*)
Patil, P.N. *et al.*, *J. Pharm. Pharmacol.*, 1967, **19**, 199, (*pharmacol*)
Britten, A.Z., *Chem. Ind. (London)*, 1968, 771, (*synth*)
Reisch, J. *et al.*, *Fresenius' Z. Anal. Chem.*, 1968, **238**, 29, (*pmr, cryst struct, deriv*)
Reisch, J. *et al.*, *J. Pharm. Pharmacol.*, 1968, **20**, 81, (*ms*)
Karoum, F. *et al.*, *Anal. Biochem.*, 1972, **47**, 550, (*glc*)
L'Hermite, P. *et al.*, *Ann. Pharm. Fr.*, 1973, **31**, 167, (*metab*)
Ger. Pat., 1973, 2 152 058; *CA*, **79**, 18354, (*pivalate*)
Kametani, T. *et al.*, *J. Het. Chem.*, 1973, **10**, 451, (*synth, cd, abs config*)
Gaglia, C.A., *Anal. Profiles Drug Subst.*, 1974, **3**, 483, (*rev*)
Brachwitz, H., *Z. Chem.*, 1974, **14**, 268, (*synth*)
Andersen, A.M., *Acta Chem. Scand., Ser. B*, 1976, **30**, 193, (*cryst struct*)
Wagner, J. *et al.*, *J. Pharm. Sci.*, 1980, **69**, 1423, (*resoln, pivalate*)
Bhaduri, D. *et al.*, *Acta Cryst. C*, 1983, **39**, 350, (*cryst struct, Phenylephrine*)
Ferguson, G. *et al.*, *Acta Cryst. C*, 1984, **40**, 1436, (*cryst struct*)
Knorr, H. *et al.*, *Arzneim.-Forsch.*, 1984, **34**, 1709, (*synth, Etilefrine*)
Eisenburger, R. *et al.*, *Arzneim.-Forsch.*, 1985, **35**, 1076, (*pivalate*)
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, 1987, 943; 1282; 1679
Midgley, J.M. *et al.*, *J.C.S. Perkin 2*, 1989, 963, (*abs config, cd, resoln*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1245; 1250; 1251
Sakuraba, S. *et al.*, *Chem. Pharm. Bull.*, 1995, **43**, 738, (*synth*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, AKT000; EGC500; EGE500; EGF000; NCL500; NNT100; SPC500