



>>Entry Name: Adiphenine, INN

Synonym(s): 2-(Diethylamino)ethyl α -phenylbenzeneacetate, 9Cl. 2-Diethylaminoethyl diphenylacetate. Adiphen. Difacil. Diphacil. Patrovina. Spasmolytin. NSC 129224

CAS Registry Number: 64-95-9

$\text{Ph}_2\text{CHCOOCH}_2\text{CH}_2\text{NEt}_2$

Molecular Formula: $\text{C}_{20}\text{H}_{25}\text{NO}_2$

Molecular Weight: 311.423

Accurate Mass: 311.188529

Percentage Composition: C 77.14%; H 8.09%; N 4.50%; O 10.28%

Biological Use/Importance: Smooth muscle relaxant, anticholinergic

Calculated Log P Data: Log P 4.35 (calc)

Hazard & Toxicity: LD_{50} (mus, orl) 600 mg/kg

>>Derivative: Hydrochloride

Synonym(s): Adiphenine hydrochloride, USAN. Paxil. Trasentine $\ddagger$. Vegantrin

CAS Registry Number: 50-42-0

Physical Description: Needles

Melting Point: Mp 113-114°

Solubility: Sol. H_2O

Hazard & Toxicity: LD_{50} (mus, orl) 500 mg/kg

Rare Chemicals Library: S42345-9

Sigma: A3649

References:

Swiss Pat., 1938, Ciba, 190 541; CA, **32**, 589, (synth)

Swiss Pat., 1938, 192 070; CA, **32**, 4174, (synth)

Swiss Pat., 1938, 192 697; CA, **32**, 4284, (synth)

Japan. Pat., 1951, 177 596; CA, **45**, 7598, (synth)

Guy, J.J. et al., J.C.S. Perkin 2, 1973, 942, (cryst struct)

Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 336

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, DHX800; THK000