



>>Entry Name: Egtazic acid, INN, USAN

Synonym(s): 3,12-Bis(carboxymethyl)-6,9-dioxa-3,12-diazatetradecanedioic acid, 9Cl. Ethylenebis(oxyethylenenitrilo)tetraacetic acid, 8Cl. Ethylene glycol bis[2-bis(carboxymethyl)amino]ethyl] ether. Ethylene glycol bis(2-aminoethyl) ether-*N,N,N',N'*-tetraacetic acid. EGTA

CAS Registry Number: 67-42-5

Type of Compound Code(s): XA3050 PA0700

(HOOCCH₂)₂NCH₂CH₂OCH₂CH₂OCH₂CH₂N(CH₂COOH)₂

Molecular Formula: C₁₄H₂₄N₂O₁₀

Molecular Weight: 380.351

Accurate Mass: 380.143098

Percentage Composition: C 44.21%; H 6.36%; N 7.37%; O 42.06%

Use/Importance: Chelating agent, e.g. used in detn. of Ca in presence of Mg. Biochemistry much investigated. Used to prepare solns. of known free Ca²⁽⁺⁾ conc. in nanomolar range

Melting Point: Mp 241 dec.°

Calculated Log P Data: Log P -1.84 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 3587 mg/kg

Aldrich: 23453-2

Fluka: 3779

Sigma: E3251

>>Derivative: Na salt

CAS Registry Number: 31571-71-8

Type of Compound Code(s): PM6700 PS8400 PS8100

Use/Importance: Used as aq. soln. as a titrant in chelatometric titration; masking agent

Physical Description: Cryst.

Solubility: Sol. H₂O, EtOH, DMF, acids, alkalis

pKa Value: pK_{a2} 2.65; pK_{a3} 8.85; pK_{a4} 9.46

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 568C, (ir)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 485B, (nmr)
U.K. Pat., 1953, 695 346; *CA*, **48**, 11486i, (manuf)
Schmid, R.W. *et al.*, *Anal. Chem.*, 1957, **29**, 264, (use)
Sudmeier, J.L. *et al.*, *Anal. Chem.*, 1964, **36**, 1698, (pmr)
Fr. Pat., 1964, 1 381 847; *CA*, **62**, 9014d, (manuf)
Wynn, J.E. *et al.*, *Toxicol. Appl. Pharmacol.*, 1970, **16**, 807, (use, tox)
Pjibil, R., *Analytical Applications of EDTA and Related Compounds*, Pergamon, Oxford, 1972, (use)
Ahamd, N. *et al.*, *Microchem. J.*, 1977, **22**, 38, (use)
Fu Chung Chang *et al.*, *Mikrochim. Acta*, 1979, **2**, 219, (masking)
Cheng, K.L. *et al.*, *Handbook of Organic Analytical Reagents*, CRC Press Boca Raton, 1982
Freeman, M.A. *et al.*, *Inorg. Chem.*, 1982, **21**, 567
Bers, D.H. *et al.*, *Am. J. Physiol.*, 1983, **242c**, 404, (detn, Ca)
Schauer, C.K. *et al.*, *Acta Cryst. C*, 1988, **44**, 981, (cryst struct, complexes)
Marks, P.W. *et al.*, *Anal. Biochem.*, 1991, **193**, 61, (use)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, EIT000