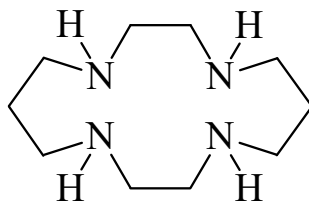




>>Entry Name: 1,4,8,11-Tetraazacyclotetradecane, 9CI

Synonym(s): Cyclam



CAS Registry Number: 295-37-4

Molecular Formula: $C_{10}H_{24}N_4$

Molecular Weight: 200.326

Accurate Mass: 200.200096

Percentage Composition: C 59.96%; H 12.08%; N 27.97%

Use/Importance: Macrocyclic ligand

Melting Point: Mp 185-186°

Aldrich: 25916-0

Fluka: 86725

Sigma: T5158

>>Derivative: 1,4,8,11-Tetrakis(2,3-dihydroxybenzoyl)

CAS Registry Number: 65950-09-6

Molecular Formula: $C_{38}H_{40}N_4O_{12}$

Molecular Weight: 744.754

Accurate Mass: 744.264276

Percentage Composition: C 61.28%; H 5.41%; N 7.52%; O 25.78%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 287 dec.°

>>Derivative: 1,8-Di-Me

Molecular Formula: $C_{12}H_{28}N_4$

Molecular Weight: 228.38

Accurate Mass: 228.231396

Percentage Composition: C 63.11%; H 12.36%; N 24.53%

Physical Description: Cryst.

Melting Point: Mp 25-30°

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **1**, 378C, (ir)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 590C, (nmr)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 470C, (ir)
Nave, C. *et al.*, *J.C.S. Dalton*, 1974, 2351-2354, (cryst struct, perchlorate)
Inorg. Synth., 1976, **16**, 220-225, (synth)
Tabushi, I. *et al.*, *Tet. Lett.*, 1977, 1049-1052, (synth)
Weitl, F.L. *et al.*, *J.A.C.S.*, 1978, **100**, 1170-1172, (synth, derivs)
Kossai, R. *et al.*, *Tet. Lett.*, 1979, 1059-1062, (synth)
Curzon, E.H. *et al.*, *J.C.S. Dalton*, 1980, 721-725, (N-15 nmr)
Org. Synth., Coll. Vol., 6, 1988, 652-662, (synth)
Helps, I.M. *et al.*, *Tetrahedron*, 1989, **45**, 219-226, (derivs)
Subramanian, S. *et al.*, *Can. J. Chem.*, 1993, **71**, 433-440, (cryst struct, complexes)
Meunier, I. *et al.*, *Can. J. Chem.*, 1995, **73**, 685-695, (synth, pmr, cmr)
Hancock, R.D. *et al.*, *J.C.S. Perkin 2*, 1996, 1925-1929, (perchlorate, cryst struct)
Comparone, A. *et al.*, *Helv. Chim. Acta*, 1998, **81**, 1765-1772, (di-Me, synth, pmr, cmr)