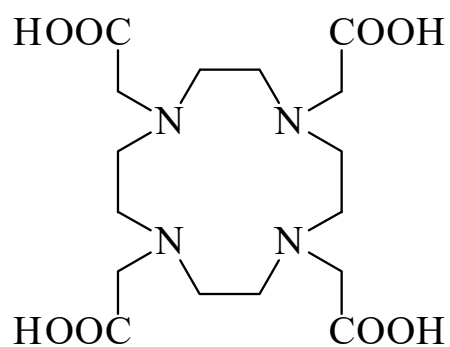




>>Entry Name: 1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetic acid, 9Cl

Synonym(s): DOTA



CAS Registry Number: 60239-18-1

Related CAS Registry Numbers(s): 60239-19-2

Molecular Formula: C₁₆H₂₈N₄O₈

Molecular Weight: 404.419

Accurate Mass: 404.190716

Percentage Composition: C 47.52%; H 6.98%; N 13.85%; O 31.65%

Use/Importance: Complexing agent

pKa Value: pK_{a1} 4.41; pK_{a2} 4.54; pK_{a3} 9.73; pK_{a4} 11.36 (20°, 0.1M KCl aq.)

Other Data: Ir 1715 cm⁻¹

>>Derivative: Hydrochloride (1:3)

CAS Registry Number: 60239-19-2

Melting Point: Mp 222 dec.°

>>Derivative: Gd(III) complex

References:

Stetter, H. *et al.*, *Angew. Chem., Int. Ed.*, 1976, **15**, 686, (*synth*)

Stetter, H. *et al.*, *Tetrahedron*, 1981, **37**, 767, (*synth*)

Riesen, A. *et al.*, *Helv. Chim. Acta*, 1986, **69**, 2067; 2074, (*complexes*)