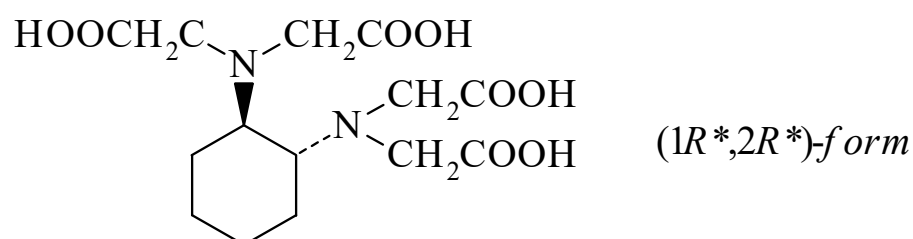




>>Entry Name: 1,2-Diaminocyclohexane-*N,N,N',N'*-tetraacetic acid

Synonym(s): *N,N'*-1,2-Cyclohexanediylbis[*N*-carboxymethylglycine], 9Cl. (1,2-Cyclohexylenedinitrilo)tetraacetic acid, 8Cl. 1,2-Cyclohexanediamine-*N,N,N',N'*-tetraacetic acid



CAS Registry Number: 482-54-2

Related CAS Registry Numbers(s): 7307-88-2 18763-65-0 28684-63-1 92761-25-6 121310-47-2 123333-90-4

Molecular Formula: C₁₄H₂₂N₂O₈

Molecular Weight: 346.336

Accurate Mass: 346.137618

Percentage Composition: C 48.55%; H 6.40%; N 8.09%; O 36.96%

Hazard & Toxicity: Irritant. LD₅₀ (rat, ipr) 413 mg/kg

>>Variant: (1*R**,2*R**)-form

Synonym(s): (+)-*trans*-form

Molecular Formula: C₁₄H₂₂N₂O₈

Molecular Weight: 346.336

Accurate Mass: 346.137618

Percentage Composition: C 48.55%; H 6.40%; N 8.09%; O 36.96%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 237°

Optical Rotation: [α]_D +53 (c, 0.5 in H₂O)

>>Variant: (1*S**,2*S**)-form

Synonym(s): (–)-*trans*-form

Molecular Formula: C₁₄H₂₂N₂O₈

Molecular Weight: 346.336

Accurate Mass: 346.137618

Percentage Composition: C 48.55%; H 6.40%; N 8.09%; O 36.96%

Physical Description: Cryst. (AcOH)

Optical Rotation: [α]_D –53 (c, 0.5 in H₂O)

>>Variant: (1*R**S*,2*R**S*)-form

Synonym(s): (±)-*trans*-form. Chelaton IV. Complexone IV. CDTA. CyDTA. DCTA

CAS Registry Number: 13291-61-7

Extra CAS Registry Numbers(s): 87095-89-4

Molecular Formula: C₁₄H₂₂N₂O₈

Molecular Weight: 346.336

Accurate Mass: 346.137618

Percentage Composition: C 48.55%; H 6.40%; N 8.09%; O 36.96%

Use/Importance: Powerful chelating agent. Complexometric titrant, masking agent; used for ion-exchange sepn. of Sr and Ba, for extraction sepn. of Cr (as anionic complex)

Physical Description: Monohydrate

Melting Point: Mp 213-216°

pKa Value: p*K*_{a2} 3.52; p*K*_{a3} 6.12; p*K*_{a4} 11.7

Other Data: Could not be resolved

Aldrich: 12581-4

Fluka: 32870

Sigma: D0922

>>Derivative: Tetra-Na salt

CAS Registry Number: 18763-65-0

Physical Description: Cryst. powder

References: