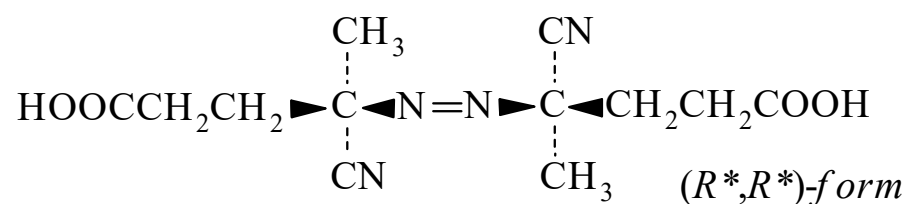




>>Entry Name: 4,4'-Azobis(4-cyanopentanoic acid), 9CI



CAS Registry Number: 2638-94-0

Molecular Formula: C₁₂H₁₆N₄O₄

Molecular Weight: 280.283

Accurate Mass: 280.117156

Percentage Composition: C 51.42%; H 5.75%; N 19.99%; O 22.83%

Use/Importance: Catalyst for radical polym.

Aldrich: 11816-8

Fluka: 11590

Sigma: A5395

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

Synonym(s): (+)-form

CAS Registry Number: 23942-62-3

Molecular Formula: C₁₂H₁₆N₄O₄

Molecular Weight: 280.283

Accurate Mass: 280.117156

Percentage Composition: C 51.42%; H 5.75%; N 19.99%; O 22.83%

Physical Description: Platelets (H₂O)

Melting Point: Mp 130-131°

Optical Rotation: [α]_D²⁵ +45.3 (c, 3.037 in MeOH)

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

Synonym(s): (–)-form

CAS Registry Number: 23886-45-5

Molecular Formula: C₁₂H₁₆N₄O₄

Molecular Weight: 280.283

Accurate Mass: 280.117156

Percentage Composition: C 51.42%; H 5.75%; N 19.99%; O 22.83%

Physical Description: Platelets (H₂O)

Melting Point: Mp 130-131°

Optical Rotation: [α]_D²⁵ –44.8 (c, 2.463 in MeOH)

>>Variant: (RS,RS)-form

Synonym(s): (±)-form

CAS Registry Number: 23886-47-7

Molecular Formula: C₁₂H₁₆N₄O₄

Molecular Weight: 280.283

Accurate Mass: 280.117156

Percentage Composition: C 51.42%; H 5.75%; N 19.99%; O 22.83%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 117-118°

>>Derivative: Dichloride

CAS Registry Number: 186266-04-6

Extra CAS Registry Numbers(s): 17170-81-9

Molecular Formula: C₁₂H₁₄Cl₂N₄O₂

Molecular Weight: 317.174

Accurate Mass: 316.04938

Percentage Composition: C 45.44%; H 4.45%; Cl 22.36%; N 17.66%; O 10.09%

Use/Importance: Intermediate for bifunctional radical initiators for alkene polymerisation

Melting Point: Mp 93-95° (88-90°)