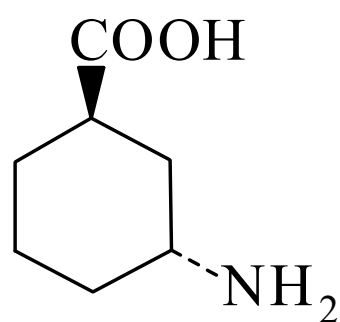




>>Entry Name: 3-Aminocyclohexanecarboxylic acid, 9CI, 8CI



(1*R* *S*,3*R* *S*)-*form*

CAS Registry Number: 25912-50-9

Molecular Formula: C₇H₁₃NO₂

Molecular Weight: 143.185

Accurate Mass: 143.094629

Percentage Composition: C 58.72%; H 9.15%; N 9.78%; O 22.35%

pKa Value: p*K*_{a1} 4.2; p*K*_{a2} 10.5 (25°)

>>Variant: (1*R*,3*R*)-form

Synonym(s): (±)-*trans*-form

Molecular Formula: C₇H₁₃NO₂

Molecular Weight: 143.185

Accurate Mass: 143.094629

Percentage Composition: C 58.72%; H 9.15%; N 9.78%; O 22.35%

Melting Point: Mp 290-291 dec.°

pKa Value: p*K*_{a1} 3.85 (15°)

>>Derivative: Benzoyl

Molecular Formula: C₁₄H₁₇NO₃

Molecular Weight: 247.293

Accurate Mass: 247.120844

Percentage Composition: C 68.00%; H 6.93%; N 5.66%; O 19.41%

Melting Point: Mp 195-196°

>>Variant: (1*R*,3*S*)-form

Synonym(s): (±)-*cis*-form

CAS Registry Number: 16636-51-4

Molecular Formula: C₇H₁₃NO₂

Molecular Weight: 143.185

Accurate Mass: 143.094629

Percentage Composition: C 58.72%; H 9.15%; N 9.78%; O 22.35%

Use/Importance: Shows anticonvulsant activity

Melting Point: Mp 284°

pKa Value: p*K*_a 3.7 (15°)

>>Derivative: Benzoyl

Melting Point: Mp 167-168°

References:

Hewgill, F.R. *et al.*, *J.C.S.*, 1955, 2767, (*synth*)

Skaric, V. *et al.*, *J.C.S. Perkin I*, 1976, 1199, (*synth*)

Murahashi, S.-I. *et al.*, *J.O.C.*, 1989, **54**, 3292, (*synth*, *pmr*)