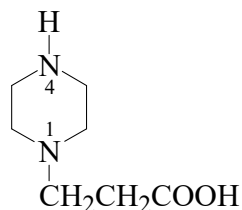




>>Entry Name: 1-Piperazinepropanoic acid, 9CI

Synonym(s): 1-(2-Carboxyethyl)piperazine



CAS Registry Number: 27245-31-4

Extra CAS Registry Numbers(s): 22278-11-1

Molecular Formula: C₇H₁₄N₂O₂

Molecular Weight: 158.2

Accurate Mass: 158.105528

Percentage Composition: C 53.15%; H 8.92%; N 17.71%; O 20.23%

Physical Description: Cryst. + ½ H₂O (MeOH) (as dihydrochloride)

Melting Point: Mp 213-216° (dihydrochloride)

>>Derivative: Me ester

CAS Registry Number: 43032-40-2

Molecular Formula: C₈H₁₆N₂O₂

Molecular Weight: 172.227

Accurate Mass: 172.121178

Percentage Composition: C 55.79%; H 9.36%; N 16.27%; O 18.58%

Physical Description: Oil

Boiling Point: Bp₁₂ 120°

>>Derivative: Me ester; hydrochloride (1:2)

CAS Registry Number: 82972-28-9

Physical Description: Cryst

Melting Point: Mp 243-244°

>>Derivative: Amide

CAS Registry Number: 5815-70-3

Molecular Formula: C₇H₁₅N₃O

Molecular Weight: 157.215

Accurate Mass: 157.121512

Percentage Composition: C 53.48%; H 9.62%; N 26.73%; O 10.18%

Physical Description: Cryst. + ½ H₂O (CHCl₃)

Melting Point: Mp 125°

>>Derivative: Nitrile

Synonym(s): *N*-(2-Cyanoethyl)piperazine

CAS Registry Number: 34064-86-3

Molecular Formula: C₇H₁₃N₃

Molecular Weight: 139.2

Accurate Mass: 139.110947

Percentage Composition: C 60.40%; H 9.41%; N 30.19%

Physical Description: Oil

Boiling Point: Bp₁₂ 135-140°

>>Derivative: 4-Me

CAS Registry Number: 55480-45-0

Molecular Formula: C₈H₁₆N₂O₂

Molecular Weight: 172.227

Accurate Mass: 172.121178

Percentage Composition: C 55.79%; H 9.36%; N 16.27%; O 18.58%

Physical Description: Cryst. (EtOH) (as dihydrochloride)

Melting Point: Mp 224-225° (dihydrochloride)