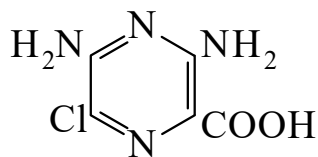




>>Entry Name: 3,5-Diamino-6-chloro-2-pyrazinecarboxylic acid



CAS Registry Number: 4878-36-8

Molecular Formula: C₅H₅ClN₄O₂

Molecular Weight: 188.573

Accurate Mass: 188.010103

Percentage Composition: C 31.85%; H 2.67%; Cl 18.80%; N 29.71%; O 16.97%

Physical Description: Cryst. (DMSO aq.)

Melting Point: Mp 272 dec.°

>>Derivative: Me ester

CAS Registry Number: 1458-01-1

Molecular Formula: C₆H₇ClN₄O₂

Molecular Weight: 202.6

Accurate Mass: 202.025753

Percentage Composition: C 35.57%; H 3.48%; Cl 17.50%; N 27.65%; O 15.79%

Physical Description: Cryst. (MeCN)

Melting Point: Mp 212-213°

>>Derivative: Amide

CAS Registry Number: 14236-57-8

Molecular Formula: C₅H₆ClN₅O

Molecular Weight: 187.588

Accurate Mass: 187.026087

Percentage Composition: C 32.01%; H 3.22%; Cl 18.90%; N 37.33%; O 8.53%

Melting Point: Mp 219-221°

Aldrich: 27788-6

Sigma: C4918

>>Derivative: Hydrazide

CAS Registry Number: 1458-11-3

Molecular Formula: C₅H₇ClN₆O

Molecular Weight: 202.603

Accurate Mass: 202.036986

Percentage Composition: C 29.64%; H 3.48%; Cl 17.50%; N 41.48%; O 7.90%

Physical Description: Cryst. (DMF aq.)

Melting Point: Mp 266-268°

>>Derivative: Nitrile

Synonym(s): 2,6-Diamino-3-chloro-6-cyanopyrazine

CAS Registry Number: 17231-59-3

Molecular Formula: C₅H₄ClN₅

Molecular Weight: 169.573

Accurate Mass: 169.015522

Percentage Composition: C 35.42%; H 2.38%; Cl 20.91%; N 41.30%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 297 dec.°

Aldrich: 30371-2

References:

- Cragoe, E.J. *et al.*, *J. Med. Chem.*, 1967, **10**, 66, (*amide, Me ester*)
Bicking, J.B. *et al.*, *J. Med. Chem.*, 1967, **10**, 598, (*Me ester*)
Jones, J.H. *et al.*, *J. Med. Chem.*, 1968, **11**, 322, (*nitrile, amide, Me ester*)
Shepard, K.L. *et al.*, *J. Med. Chem.*, 1969, **12**, 280, (*synth, anal, props*)
Smith, R.L. *et al.*, *J.A.C.S.*, 1979, **101**, 191, (*amide, pmr*)