



Formula: C3H2ClN3O2

MW: 147.52

CAS: 57531-37-0

MDL NUMBER: MFCD03419295

IUPAC: 2-chloro-4-nitroimidazole

Smiles: c1(c[nH]c(n1)Cl)[N+](=[O-])=O

THERAPEUTIC CATEGORY: anti amoebic

ACCEPTORS: 2

DONORS: 1

ROTATION BONDS: 0

N+O: 5

Chiral Centers: 0

LogP: 0.49

LogS: -2.48

LIPINSKI: 4

Synonyms: TIMTEC-BB SBB000100;1H-IMIDAZOLE,  
2-CHLORO-4-NITRO-;2-CHLORO-5-NITRO-1H-IMIDAZOLE;2-CHLORO-4-NITROIMIDAZOLE;  
2-Chloro-4-nitro-1H-imidazole;1H-Imidazole,2-chloro-4-nitro-(9CI);2-CHLORO-4-NITRO-1H-IMI  
DAZOLE, 98+%;2-Chloro-5-nitroimidazole

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EINECS:

Product Categories:NITRO;Halides;Imidazoles & Benzimidazoles;API intermediates;Imidazoles  
& Benzimidazoles 2-Chloro-4-nitroimidazole

Chemical Properties:

CAS DataBase Reference: 57531-37-0(

CAS DataBase Reference: ) Xi Risk Statements 36/37/38 Safety Statements 26-36  
HazardClass IRRITANT 2-Chloro-4-nitroimidazole

Usage And Synthesis: 2-Chloro-4-nitroimidazole

