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Typical Product Specifications & Properties

Benzonitrile, 2-chloro-5-nitro-

CAS Number: : 16588-02-6

Specifications	Limits
Chemical Structure	 chemicalStructure-benzonitrile-2-chloro-5-nitro-
Chemical Structure	 615826 615826_benzonitrile-2-chloro-5-nitro-.png chemical structure
Molecular Formula	C7H3ClN2O2
Molecular weight	
Canonicalized Compound	1
Compound Complexity	229
Hydrogen Bond Acceptor Count	3
Hydrogen Bond Donor Count	
Rotatable Bond Count	
Allowed IUPAC Name	2-chloro-5-nitro-benzonitrile
CAS-like Style IUPAC Name	2-chloro-5-nitrobenzonitrile
Markup IUPAC Name	2-chloro-5-nitrobenzonitrile



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Specifications	Limits
Preferred IUPAC Name	2-chloro-5-nitrobenzonitrile
Systematic IUPAC Name	2-chloranyl-5-nitro-benzenecarbonitrile
Traditional IUPAC Name	2-chloro-5-nitro-benzonitrile
Standard InChI	InChI=1S/C7H3ClN2O2/c8-7-2-1-6(10(11)12)3-5(7)4-9/h1-3H
Standard InChIKey	ZGILLTVEEBNDOB-UHFFFAOYSA-N
Exact Mass	181.9883050
Molecular Weight	182.56
Canonical SMILES	<chem>C1=CC(=C(C=C1[N+](=O)[O-])C#N)Cl</chem>
Isomeric SMILES	<chem>C1=CC(=C(C=C1[N+](=O)[O-])C#N)Cl</chem>
Polar Surface Area Topological	69.6
Monoisotopic Weight	181.9883050
XLogP3 Log P	2.2



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