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## Typical Product Specifications & Properties

# 2-Aminomethyl-3-chloropyrazine HCl

CAS Number: : 22680-44-0

| Specifications            | Limits  |
|---------------------------|---|
| Allowed IUPAC Name        | (2-chlorophenyl)methanamine;hydrochloride                 |
| CAS-like Style IUPAC Name | (2-chlorophenyl)methanamine;hydrochloride                 |
| Markup IUPAC Name         | (2-chlorophenyl)methanamine;hydrochloride                 |
| Preferred IUPAC Name      | (2-chlorophenyl)methanamine;hydrochloride                 |
| Systematic IUPAC Name     | (2-chlorophenyl)methanamine;hydrochloride                 |
| Traditional IUPAC Name    | (2-chlorobenzyl)amine;hydrochloride                       |
| Standard InChI            | InChI=1S/C7H8ClN.ClH/c8-7-4-2-1-3-6(7)5-9;/h1-4H,5,9H2;1H |
| Standard InChIKey         | LXFIZCSCVYTFBU-UHFFFAOYSA-N                               |
| Exact Mass                | 177.0112047   |
| Molecular Weight          | 178.06  |
| Canonical SMILES          | <chem>C1=CC=C(C(=C1)CN)Cl.Cl</chem>                       |
| Isomeric SMILES           | <chem>C1=CC=C(C(=C1)CN)Cl.Cl</chem>                       |



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| Specifications                 | Limits   |
|--------------------------------|--|
| Polar Surface Area Topological | 26   |
| Monoisotopic Weight            | 177.0112047  |
| Molecular Formula              | C7H9Cl2N   |
| Molecular weight               |  |
| Canonicalized Compound         | 1  |
| Compound Complexity            | 85   |
| Hydrogen Bond Acceptor Count   | 1  |
| Hydrogen Bond Donor Count      | 2  |
| Rotatable Bond Count           | 1  |
| Chemical Structure             |  chemicalStructure-2-aminomethyl-3-chloropyrazine-hcl |



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