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Typical Product Specifications & Properties

Isoquinoline-1-carboxylic Acid

CAS Number: : 486-73-7

Specifications	Limits
Molecular weight	173.17
EINECS	207-639-6
InChI	1S/C10H7NO2/c12-10(13)9-8-4-2-1-3-7(8)5-6-11-9/h1-6H,(H,12,13)
InChIKey	XAAKCCMYRKZRAK-UHFFFAOYSA-N
Refractive Index	1.358
Melting Point	164 °C (dec.)
BRN Number	129177
Density	0.932 g/mL at 20 °C
Storage Temperature	0-6°C
Merck	13,9784
Boiling Point	68-69 °C
Flash Point	8 °F



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Specifications	Limits
Vapor Density	3.59
Molecular weight	164.95
EINECS	204-828-5
SMILES	[Na+].CC(Cl)(Cl)C(=O)[O-]
InChI	PDEFQWNXOUGDJR-UHFFFAOYSA-M
InChIKey	1S/C3H4Cl2O2.Na/c1-3(4,5)2(6)7;/h1H3,(H,6,7);/q;+1/p-1
Storage Temperature	+4°C
Molecular weight	122.17
EINECS	207-826-2
SMILES	c1(c(ccc(c1)C)N)N
InChI	1S/C7H10N2/c1-5-2-3-6(8)7(9)4-5/h2-4H,8-9H2,1H3
InChIKey	DGRGLKZMKWPMOH-UHFFFAOYSA-N



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Specifications	Limits
Stability	Stable. Incompatible with strong oxidizing agents.
Flash Point	155-156°C/18mm
Melting Point	87-89 °C
BRN Number	507965
Boiling Point	155-156 °C18 mm Hg

Specifications	Limits
Water solubility	16 g/L (20 °C)



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