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Typical Product Specifications & Properties

3-Iodopyridine-2-carbonitrile

CAS Number: : 827616-52-4

| Specifications | Limits |
|------------------|---|
| Molecular weight | 230.01 |
| Molecular weight | 250.25 |
| SMILES | <chem>c1cc(ccc1Cc2ccc(cc2)N=C=O)N=C=O</chem> |
| InChI | 1S/C15H10N2O2/c18-10-16-14-5-1-12(2-6-14)9-13-3-7-15(8-4-13)17-11-19/h1-8H,9H2 |
| InChIKey | UPMLOUAZCHDJJD-UHFFFAOYSA-N |
| Flash Point | 196 °C |
| Boiling Point | 392 °C |
| Density | 1.19 |
| Melting Point | 38-44 °C |
| BRN Number | 797662 |
| Water solubility | decomposes |
| Stability | Stable. Combustible. Incompatible with strong oxidizing agents. Reacts violently with alcohols. |





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| Specifications | Limits |
|------------------------------|--|
| Sensitive | Moisture Sensitive/Lachrymatory |
| Freezing Point | 37? |
| Storage Temperature | Refrigerator |
| Freezing Point | 37? |
| Vapor Pressure | 5.00E-06 mm Hg |
| Henry's Law Constant | 8.95E-07 atm-m ³ /mole |
| Melting Point | 38 ° C |
| log P (octanol-water) | 5.220 |
| Water solubility | 0.829 mg/L |
| Atmospheric OH Rate Constant | 1.20E-11 cm ³ /molecule-sec |
| Freezing Point | 37? |



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415 Huguenot Street, New Rochelle, New York 10801

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