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Typical Product Specifications & Properties

3-Nitrobenzotrifluoride

CAS Number: : 98-46-4

Specifications	Limits
Molecular weight	191.11
EINECS	202-670-1
SMILES	<chem>c1(cc(ccc1)[N+](=O)[O-])C(F)(F)F</chem>
InChI	1S/C7H4F3NO2/c8-7(9,10)5-2-1-3-6(4-5)11(12)13/h1-4H
InChIKey	WHNAMGUAXHGCHH-UHFFFAOYSA-N
Vapor Pressure	0.259 mm Hg
Water solubility	114 mg/L
Melting Point	-2.40E+00 ° C
Boiling Point	202.8 ° C
log P (octanol-water)	2.62
Atmospheric OH Rate Constant	4.90E-14 cm ³ /molecule-sec
Henry's Law Constant	1.85E-04 atm-m ³ /mole



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Specifications	Limits
Boiling Point	200-205 °C
BRN Number	2051362
Density	1.436 g/mL at 25 °C
Melting Point	-5 °C
Water solubility	0.4 g/L (20 °C)
Refractive Index	1.472
Flash Point	190 °F



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