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Typical Product Specifications & Properties

1,3,5-Trinitrobenzene

CAS Number: : 99-35-4

Specifications	Limits
Molecular weight	213.10
EINECS	202-752-7
SMILES	<chem>c1(cc(cc(c1)[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]</chem>
InChI	1S/C6H3N3O6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H
InChIKey	UATJOMSPNYCXIX-UHFFFAOYSA-N
Boiling Point	315 ° C
log P (octanol-water)	1.18
Atmospheric OH Rate Constant	1.30E-15 cm ³ /molecule-sec
Henry's Law Constant	3.31E-10 atm-m ³ /mole
Water solubility	278 mg/L
Melting Point	121.5 ° C
Melting Point	122°C



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Specifications	Limits
Storage Temperature	2-8°C
Merck	9726



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