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Typical Product Specifications & Properties

Isoamyl Nitrate

CAS Number: : 543-87-3

Specifications	Limits
Molecular weight	133.15
EINECS	208-852-7
SMILES	<chem>C(CCO[N+](O)=O)(C)C</chem>
InChI	1S/C5H11NO3/c1-5(2)3-4-9-6(7)8/h5H,3-4H2,1-2H3
InChIKey	NT HGIYFSMNNHSC-UHFFFAOYSA-N
log P (octanol-water)	2.84
Vapor Pressure	5.440 mm Hg
Boiling Point	148 ° C
Melting Point	0.0 ° C
Water solubility	440 mg/L
Henry's Law Constant	0.0022 atm-m ³ /mole
Atmospheric OH Rate Constant	3.36E-12 cm ³ /molecule-sec



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Specifications	Limits
Density	1.00
Flash Point	49?
Boiling Point	148 °C
Refractive Index	1.4110-1.4140
Merck	5122



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