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## Typical Product Specifications & Properties

# Thionicotinamide

CAS Number: : 4621-66-3

Specifications	Limits
Molecular weight	138.19
SMILES	<chem>c1(cccnc1)C(N)=S</chem>
InChI	XQWBMZ WDJAZ PPX-UHFFFAOYSA-N
InChIKey	1S/C6H6N2S/c7-6(9)5-2-1-3-8-4-5/h1-4H,(H2,7,9)
Vapor Pressure	8.41E-03 mm Hg
Atmospheric OH Rate Constant	2.18E-11 cm <sup>3</sup> /molecule-sec
Water solubility	2.32E+05 mg/L
Henry's Law Constant	5.13E-10 atm-m <sup>3</sup> /mole
log P (octanol-water)	0.67



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