

## Typical Product Specifications & Properties

# 4-Chlorophenyl isothiocyanate

CAS Number: : 2131-55-7

Specifications	Limits
Molecular weight	169.63
SMILES	<chem>c1(ccc(Cl)cc1)N=C=S</chem>
InChI	1S/C7H4ClNS/c8-6-1-3-7(4-2-6)9-5-10/h1-4H
InChIKey	MZZVFXMTZTVUFO-UHFFFAOYSA-N
Melting Point	46 &deg; C
Boiling Point	249.5 &deg; C
Atmospheric OH Rate Constant	1.50E-12 cm <sup>3</sup> /molecule-sec
Water solubility	28.3 mg/L
Vapor Pressure	0.013 mm Hg
Henry's Law Constant	5.79E-04 atm-m <sup>3</sup> /mole
log P (octanol-water)	3.91