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## Typical Product Specifications & Properties

# Thiamine pyrophosphate chloride

CAS Number: : 154-87-0

Specifications	Limits
Molecular weight	460.77
EINECS	205-230-7
SMILES	<chem>[n+]1(c(c(CCO[P@@](OP(O)(O)=O)(O)=O)sc1)C)Cc1c(nc(C)nc1)N.[Cl-]</chem>
InChI	YXVCLPJQTZXJLH-UHFFFAOYSA-N
InChIKey	1S/C12H18N4O7P2S.ClH/c1-8-11(3-4-22-25(20,21)23-24(17,18)19)26-7-16(8)6-10-5-14-9(2)15-12(10)13;/h5,7H,3-4,6H2,1-2H3,(H4-,13,14,15,17,18,19,20,21);1H
Atmospheric OH Rate Constant	2.96E-11 cm <sup>3</sup> /molecule-sec
log P (octanol-water)	-0.100
Water solubility	It is soluble in water.
Storage Temperature	2-8&deg;C



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