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Typical Product Specifications & Properties

9H-Purine-9-Acetic Acid, 6-[(P-Chlorophenyl)Amino]-, Ethyl Ester

CAS Number: : 101103-22-4

Specifications	Limits
Molecular weight	331.76
InChI	1S/C15H14ClN5O2/c1-2-23-12(22)7-21-9-19-13-14(17-8-18-15(13)21)20-11-5-3-10(16)4-6-11/h3-6,8-9H,2,7H2,1H3,(H,17,18,20)
InChIKey	GRZHGZVUENNXNQ-UHFFFAOYSA-N
Molecular weight	275.52
EINECS	202-910-5
SMILES	c1(Nc2c(cccc2)Cl)nc(nc(n1)Cl)Cl
InChI	1S/C9H5Cl3N4/c10-5-3-1-2-4-6(5)13-9-15-7(11)14-8(12)16-9/h1-4H,(H,13,14,15,16)
InChIKey	IMHBYKMAHXWHRP-UHFFFAOYSA-N
log P (octanol-water)	3.88
Water solubility	8 mg/L
Atmospheric OH Rate Constant	4.28E-11 cm ³ /molecule-sec
Vapor Pressure	6.20E-09 mm Hg



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Specifications	Limits
Henry's Law Constant	2.81E-10 atm-m ³ /mole
Melting Point	160 ° C



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