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Typical Product Specifications & Properties

1H-Purine-2,6(3H,7H)-dione

CAS Number: : 69-89-6

Specifications	Limits
Molecular weight	152.11
SMILES	<chem>c12c(c([nH]c([nH]1)=O)=O)[nH]cn2</chem>
InChI	1S/C5H4N4O2/c10-4-2-3(7-1-6-2)8-5(11)9-4/h1H,(H3,6,7,8,9,10,11)
InChIKey	LRFVTYWOQMYALW-UHFFFAOYSA-N
pKa Dissociation Constant	7.53
Vapor Pressure	2.64E-10 mm Hg
Atmospheric OH Rate Constant	5.48E-11 cm ³ /molecule-sec
Water solubility	69 mg/L
log P (octanol-water)	-0.73
Henry's Law Constant	3.73E-14 atm-m ³ /mole



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