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Typical Product Specifications & Properties

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

CAS Number: : 603-00-9

Specifications	Limits
Molecular weight	238.24
EINECS	210-028-7
SMILES	<chem>CC(Cn1cnc2c1c(=O)n(c(=O)n2C)C)O</chem>
InChI	1S/C10H14N4O3/c1-6(15)4-14-5-11-8-7(14)9(16)13(3)10(17)12(8)2/h5-6,15H,4H2,1-3H3
InChIKey	KYHQZNGJUGFTGR-UHFFFAOYSA-N
Atmospheric OH Rate Constant	2.91E-11 cm ³ /molecule-sec
log P (octanol-water)	-0.77
Melting Point	135.5 ° C
Vapor Pressure	5.66E-12 mm Hg
Water solubility	1.00E+06 mg/L
Henry's Law Constant	2.31E-15 atm-m ³ /mole



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