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Typical Product Specifications & Properties

7-Methylxanthine

CAS Number: : 552-62-5

Specifications	Limits
Molecular weight	166.14
InChI	1S/C6H6N4O2/c1-10-2-7-4-3(10)5(11)9-6(12)8-4/h2H,1H3,(H2,8,9,11,12)
InChIKey	PFWLFWPASULGAN-UHFFFAOYSA-N
Water solubility	1.81E+04 mg/L
Henry's Law Constant	7.95E-13 atm-m3/mole
Atmospheric OH Rate Constant	5.49E-11 cm3/molecule-sec
Vapor Pressure	1.88E-09 mm Hg
log P (octanol-water)	-0.89
Melting Point	> 300 ° C
pKa Dissociation Constant	8.33



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