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Typical Product Specifications & Properties

3-Isobutyl-1-methylxanthine

CAS Number: : 28822-58-4

Specifications	Limits
Molecular weight	222.24
EINECS	249-259-3
InChI	1S/C10H14N4O2/c1-6(2)4-14-8-7(11-5-12-8)9(15)13(3)10(14)16/h5-6H,4H2,1-3H3,(H,11,12)
InChIKey	APIXJSLKIYYUKG-UHFFFAOYSA-N
Melting Point	200-201 °C
Henry's Law Constant	3.92E-12 atm-m ³ /mole
log P (octanol-water)	1.15
Vapor Pressure	7.25E-10 mm Hg
Atmospheric OH Rate Constant	2.62E-11 cm ³ /molecule-sec
Water solubility	3490 mg/L
Form	powder
Storage Temperature	-20°C



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Specifications	Limits
Solubility	DMSO: 1 M with gentle warming
Melting Point	200-201 °C
Color	off-white
Storage Temperature	-20°C
Storage Temperature	-20°C



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