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Typical Product Specifications & Properties

1-n-Hexyltheobromine

CAS Number: : 1028-33-7

Specifications	Limits
Molecular weight	264.32
InChI	1S/C13H20N4O2/c1-4-5-6-7-8-17-12(18)10-11(14-9-15(10)2)16(3)13(17)19/h9H,4-8H2,1-3H3
InChIKey	MRWQRJMESRRJJB-UHFFFAOYSA-N
log P (octanol-water)	2.610
Vapor Pressure	6.11E-10 mm Hg
Water solubility	116 mg/L
Henry's Law Constant	1.48E-10 atm-m ³ /mole
Melting Point	82.5 ° C
Atmospheric OH Rate Constant	2.91E-11 cm ³ /molecule-sec



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