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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-m3/mole                                                                 |
| Melting Point                | 82.5 &deg; C                                                                         |
| Atmospheric OH Rate Constant | 2.91E-11 cm3/molecule-sec                                                            |



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