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Typical Product Specifications & Properties

1,3,7-Trimethyl-7,9-Dihydro-1H-Purine-2,6,8(3H)-Trione

CAS Number: : 5415-44-1

| Specifications | Limits |
|------------------------------|--|
| Molecular weight | 210.19 |
| EINECS | 226-507-9 |
| SMILES | <chem>Cn1c(=O)n(C)c2[nH]c(=O)n(c2c1=O)C</chem> |
| InChI | 1S/C8H10N4O3/c1-10-4-5(9-7(10)14)11(2)8(15)12(3)6(4)13/h1-3H3,(H,9,14) |
| InChIKey | BYXCFUMGEBZDDI-UHFFFAOYSA-N |
| log P (octanol-water) | -0.37 |
| Vapor Pressure | 7.23E-09 mm Hg |
| pKa Dissociation Constant | 6 |
| Atmospheric OH Rate Constant | 1.40E-11 cm ³ /molecule-sec |
| Water solubility | 5500 mg/L |
| Henry's Law Constant | 1.27E-16 atm-m ³ /mole |



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