

Typical Product Specifications & Properties

2-(1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-7H-purin-7-yl)ethyl nicotinate

CAS Number: : 13425-39-3

Specifications	Limits
Molecular weight	329.31
EINECS	236-544-2
SMILES	<chem>Cn1c2c(c(=O)n(c1=O)C)n(cn2)CCOC(=O)c3cccnc3</chem>
InChI	ZWIAODBBEZGVPY-UHFFFAOYSA-N
InChIKey	1S/C15H15N5O4/c1-18-12-11(13(21)19(2)15(18)23)20(9-17-12)6-7-24-14(22)10-4-3-5-16-8-10/h3-5,8-9H,6-7H2,1-2H3
Atmospheric OH Rate Constant	2.24E-11 cm ³ /molecule-sec
Henry's Law Constant	2.93E-17 atm-m ³ /mole
Melting Point	151-152 °C
Water solubility	2.00E+04 mg/L
Vapor Pressure	1.84E-12 mm Hg
log P (octanol-water)	0.450