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Typical Product Specifications & Properties

Xanthine Amine Congener

CAS Number: : 96865-92-8

Specifications	Limits
Molecular weight	428.48
SMILES	<chem>c12c(c(n(CCC)c(n1CCC)=O)=O)[nH]c(n2)c1ccc(OCC(=O)NCCN)cc1</chem>
InChI	FIQGIOAELHTLHM-UHFFFAOYSA-N
InChIKey	1S/C21H28N6O4/c1-3-11-26-19-17(20(29)27(12-4-2)21(26)30)24-18(25-19)14-5-7-15(8-6-14)31-13-16(28)23-10-9-22/h5-8H,3-4,9-13,22H2,1-2H3,(H,23,28)(H,24,25)



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