

## Typical Product Specifications & Properties

# 7-(2-Chloroethyl)theophylline

CAS Number: : 5878-61-5

Specifications	Limits
Molecular weight	242.66
SMILES	<chem>Cn1c2c(c(=O)n(c1=O)C)n(cn2)CCCl</chem>
InChI	QCIARNIKNKKHFH-UHFFFAOYSA-N
InChIKey	1S/C9H11ClN4O2/c1-12-7-6(8(15)13(2)9(12)16)14(4-3-10)5-11-7/h5H,3-4H2,1-2H3