9H-purine, 6-chloro-2,9-diethyl

InChI: InChI=1S/C9H11ClN4/c1-3-6-12-8(10)7-9(13-6)14(4-2)5-11-7/h5H,3-4H2,1-2H3

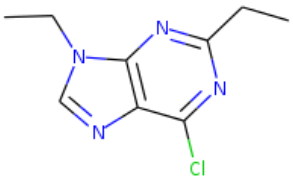
InChI Key: WZHZKKOJBLGUPI-UHFFFAOYSA-N

Formula: C9H11ClN4

SMILES: CCc1nc2c(ncn2CC)c(Cl)n1

Molecular Weight: 210.66

CAS: 5466-13-7



Physical Properties

Property	Value	Unit	Source
*log*P$_{oct/wat}$	2.06		Crippen Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H11ClN4/c1-3-6-12-8(10)7-9(13-6)14(4-2)5-11-7/h5H,3-4H2,1-2H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

***log*P$_{oct/wat}$**: Octanol/Water partition coefficient .