

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

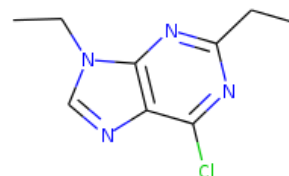
InChI Key: WZHZZKQJBLGUPI-UHFFFAOYSA-N

Formula: C₉H₁₁ClN₄

SMILES: CCc1nc2c(ncn2CC)c(Cl)n1

Molecular Weight: 210.66

CAS: 5466-13-7



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	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](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/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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