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
InchiKey: WZHZKKOJBLGUPI-UHFFFAOYSA-N
Formula: C9H11ClN4
SMILES: CCc1nc(Cl)c2ncn(CC)c2n1
Mol. weight [g/mol]: 210.66
CAS: 5466-13-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.32		Crippen Method
logp	2.062		Crippen Method
mcvol	150.910	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5466137&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume