2-Chloro-6-dimethylaminopurine

Inchi: InChI=1S/C7H8ClN5/c1-13(2)6-4-5(10-3-9-4)11-7(8)12-6/h3H,1-2H3,(H,9,10,11,12)
InchiKey: BJAYANZFEQNNDV-UHFFFAOYSA-N
Formula: C7H8ClN5
SMILES: CN(C)c1nc(Cl)nc2nc[nH]c12
Mol. weight [g/mol]: 197.62
CAS: 100960-20-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	0.590		Crippen Method
mcvol	132.710	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100960201&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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