9H-purine, 6-chloro-9-(2-chloroethyl)-

Inchi: InChI=1S/C7H6Cl2N4/c8-1-2-13-4-12-5-6(9)10-3-11-7(5)13/h3-4H,1-2H2
InchiKey: BLBSNXLJIBKTOJ-UHFFFAOYSA-N
Formula: C7H6Cl2N4
SMILES: ClCCn1cnc2c(Cl)ncnc21
Mol. weight [g/mol]: 217.06
CAS: 64127-00-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	1.719		Crippen Method
mcvol	134.970	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=C64127000&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