

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

Latest version available from:

<https://www.chemeo.com/cid/66-646-2/9H-purine-6-chloro-9-2-chloroethyl.pdf>

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