

9H-purine, 6-chloro-9-ethyl-

Inchi:	InChI=1S/C7H7ClN4/c1-2-12-4-11-5-6(8)9-3-10-7(5)12/h3-4H,2H2,1H3
InchiKey:	YSKHRCGNQFWRFM-UHFFFAOYSA-N
Formula:	C7H7ClN4
SMILES:	CCn1cnc2c(Cl)ncnc21
Mol. weight [g/mol]:	182.61
CAS:	5462-86-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	1.500		Crippen Method
mcvol	122.730	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5462862&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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