

Cyclohexanol, 2-(9h-6-chloropurin-9-yl)-, trans

Inchi:	InChI=1S/C11H13ClN4O/c12-10-9-11(14-5-13-10)16(6-15-9)7-3-1-2-4-8(7)17/h5-8,17H,1
InchiKey:	CKTCXOLCNXSTKZ-UHFFFAOYSA-N
Formula:	C11H13ClN4O
SMILES:	OC1CCCCC1n1cnc2c(Cl)ncnc21
Mol. weight [g/mol]:	252.70
CAS:	5463-96-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.43		Crippen Method
logp	1.956		Crippen Method
mcvol	174.100	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=C5463967&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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