6-Chloropurine

Other names:	1H-Purine, 6-chloro-
	6-CP
	6-Chloro-1H-purine
	6-Chloro-9H-purine
	6-Chlorpurine
	6-chloro-7H-purine
	ClP
	NSC 744
	Purine, 6-chloro-
	SK 6048
	X 47
Inchi:	InChI=1S/C5H3ClN4/c6-4-3-5(9-1-7-3)10-2-8-4/h1-2H,(H,7,8,9,10)
InchiKey:	ZKBQDFAWXLTYKS-UHFFFAOYSA-N
Formula:	C5H3ClN4
SMILES:	Clc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	154.56
CAS:	87-42-3

Physical Properties

Property code	Value	Unit	Source
affp	873.60	kJ/mol	NIST Webbook
basg	841.70	kJ/mol	NIST Webbook
log10ws	-2.48		Crippen Method
logp	0.524		Crippen Method
mcvol	94.550	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87423&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility modelling, solvent effect and preferential solvation of 6-chloropurine in several aqueous co-solvent mixtures between 283.15 K and 328.15 K:	https://www.doi.org/10.1016/j.jct.2018.07.028
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume