

Guanazine

Other names:	[1,2,4]Triazole-3,4,5-triamine 3,4,5-triamino-1,2,4-triazole
Inchi:	InChI=1S/C2H6N6/c3-1-6-7-2(4)8(1)5/h5H2,(H2,3,6)(H2,4,7)
InchiKey:	JJGGIYYGVKGMQZ-UHFFFAOYSA-N
Formula:	C2H6N6
SMILES:	N=c1[nH][nH]c(=N)n1N
Mol. weight [g/mol]:	114.11
CAS:	473-96-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.98		Crippen Method
logp	-3.147		Crippen Method
mcvol	79.460	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C473961&Units=SI

Legend

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

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