1,3,5-Triazine-2,4-diamine, 6-chloro-

Other names:	s-Triazine, 2,4-diamino-6-chloro-
	ENT 50982
	G 28273
	2-Chloro-4,6-diamino-1,3,5-triazine
	2-Chloro-4,6-diaminotriazine
	2,4-Diamino-6-chloro-1,3,5-triazine
	6-Chloro-1,3,5-triazine-2,4-diamine
	Simazine di-dealkylated
	Desethyl-desisopropyl-atrazine
	2-Chloro-4,6-diamino-s-triazine
	NSC 680830
	NSC 7965
	Atrazine M (des-ethyl, des-isopropyl)
Inchi:	InChI=1S/C3H4ClN5/c4-1-7-2(5)9-3(6)8-1/h(H4,5,6,7,8,9)
InchiKey:	FVFVNNKYKYZTJU-UHFFFAOYSA-N
Formula:	C3H4ClN5
SMILES:	N=c1nc(Cl)[nH]c(=N)[nH]1
Mol. weight [g/mol]:	145.55
CAS:	3397-62-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	-1.614		Crippen Method
mcvol	91.510	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=C3397624&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