

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:	FVFNKYKYZTJU-UHFFFAOYSA-N
Formula:	C3H4ClN5
SMILES:	<chem>N=c1nc(Cl)[nH]c(=N)[nH]1</chem>
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
mcpvol	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

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