

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

Other names:	s-Triazine, 2-amino-4-chloro-6-(ethylamino)- G 28279 Atrazine deisopropyl Atrazine, desisopropyl Deisopropylatrazine Desethylsimazine Desisopropylatrazine Simazine, desethyl Atrazine M (des-isopropyl)
Inchi:	InChI=1S/C5H8ClN5/c1-2-8-5-10-3(6)9-4(7)11-5/h2H2,1H3,(H3,7,8,9,10,11)
InchiKey:	IVENSCMCQBIAKW-UHFFFAOYSA-N
Formula:	C5H8ClN5
SMILES:	CCNc1nc(N)nc(Cl)n1
Mol. weight [g/mol]:	173.60
CAS:	1007-28-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.52		Crippen Method
logp	0.539		Crippen Method
mcvol	119.690	ml/mol	McGowan Method
rinpol	1654.00		NIST Webbook
rinpol	280.28		NIST Webbook
rinpol	280.28		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1007289&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/49-847-8/1-3-5-Triazine-2-4-diamine-6-chloro-N-ethyl.pdf>

Generated by Cheméo on 2024-04-20 03:10:52.445756662 +0000 UTC m=+15871901.366333978.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.