

6-Chloro-N,N'-(1-methylpropyl)-[1,3,5]triazine-2,4-

Inchi:	InChI=1S/C11H20ClN5/c1-5-7(3)13-10-15-9(12)16-11(17-10)14-8(4)6-2/h7-8H,5-6H2,1-4H
InchiKey:	NTYCDOAJCGVIMP-UHFFFAOYSA-N
Formula:	C11H20ClN5
SMILES:	CCC(C)N=c1nc(Cl)[nH]c(=NC(C)CC)[nH]1
Mol. weight [g/mol]:	257.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	0.826		Crippen Method
mcvol	204.230	ml/mol	McGowan Method
rinpol	1918.11		NIST Webbook
rinpol	1929.42		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=R288672&Units=SI

Legend

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

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