

6-Chloro-N-sec-butyl-1,3,5-triazine-2,4-diamine

Other names:	N-sec-Butyl-6-chloro-1,3,5-triazine-2,4-diamine Desethylsebutylazine Sebuthylazin-desethyl
Inchi:	InChI=1S/C7H12ClN5/c1-3-4(2)10-7-12-5(8)11-6(9)13-7/h4H,3H2,1-2H3,(H3,9,10,11,12,
InchiKey:	VMYDDULRGBGGBN-UHFFFAOYSA-N
Formula:	C7H12ClN5
SMILES:	CCC(C)Nc1nc(N)nc(Cl)n1
Mol. weight [g/mol]:	201.66
CAS:	37019-18-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	1.318		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
rmpol	1780.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37019184&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
rmpol:	Non-polar retention indices

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