N-tert-Butyl-6-chlor-[1,3,5]triazin-2,4-diamine

Other names:	1,3,5-Triazine-2,4-diamine, 6-chloro-N-(1,1-dimethylethyl)- 6-Chloro-N-(1,1-dimethylethyl)-1,3,5-triazine-2,4-diamine N-tert-Butyl-6-chlor-[1,3,5]triazin-2,4-diamine N-tert-Butyl-6-chloro-[1,3,5]triazinane-2,4-diamine Terbuthylazine (des-ethyl) Terbuthylazine M (des-ethyl)
Inchi:	InChI=1S/C7H12ClN5/c1-7(2,3)13-6-11-4(8)10-5(9)12-6/h1-3H3,(H3,9,10,11,12,13)
InchiKey:	LMKQNTMFZLAJDV-UHFFFAOYSA-N
Formula:	C7H12ClN5
SMILES:	CC(C)(C)Nc1nc(N)nc(Cl)n1
Mol. weight [g/mol]:	201.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.91		Cheméo Relay (1.0)
logp	1.318		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
tf	487.75	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30125634&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point