Desethylterbutylazine

Other names:	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)
	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
	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
CAS:	30125-63-4

Physical Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30125634&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Latest version available from:

https://www.chemeo.com/cid/25-777-2/Desethylterbutylazine.pdf

Generated by Cheméo on 2024-10-12 06:34:21.888331441 +0000 UTC m=+3295724.525300692.

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