N-tert-Butyl-N'-acetyl-N'-cyclopropyl-6-methylsulf

Other names:	N-Acetyl-N-Cyclopropyl-N'-(2-methyl-2-propanyl)-6-(methylsulfanyl)-1,3,5-triazine-2,4-dia
	2-(tert-Butylamino)-4-(cyclopropyl-acetylamino)-6-(methylthio)-s-triazine
	2-Methylthio-4-tert-butylamino-6-cyclopropyl-acetylamino-S-triazine
	N2-tert-Butyl-N4-acetyl-N4-cyclopropyl-6-methylthio-1,3,5-triazine-2,4-diamine
	N'-t-Butyl-N-acetyl-N-cyclopropyl-6-(methylthio)-1,3,5-triazine-2,4-diamine
Inchi:	InChI=1S/C13H21N5OS/c1-8(19)18(9-6-7-9)11-14-10(17-13(2,3)4)15-12(16-11)20-5/h9H
InchiKey:	DAZIASGCGUZIAP-UHFFFAOYSA-N
Formula:	C13H21N5OS
SMILES:	CSc1nc(NC(C)(C)C)nc(N(C(C)=O)C2CC2)n1
Mol. weight [g/mol]:	295.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	2.319		Crippen Method
mcvol	227.230	ml/mol	McGowan Method
rinpol	2248.00		NIST Webbook
rinpol	2248.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.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=U373131&Units=SI
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

rinpol: Non-polar retention indices