N-tert-Butyl-N'-acetyl-6-methoxy-1,3,5-triazine-2,4

Other names: 2-Acetylamino-4-tert-butylamino-6-methoxy-1,3,5-triazine
6-Methoxy-N-(2-methyl-2-propanyl)-N'-acetyl-1,3,5-triazin-2,4-diamin
Inchi: InChI=1S/C10H17N5O2/c1-6(16)11-7-12-8(15-10(2,3)4)14-9(13-7)17-5/h1-5H3,(H2,11,1
InchiKey: ZYRYLSPHDLCOKO-UHFFFAOYSA-N
Formula: C10H17N5O2
SMILES: COc1nc(NC(C)=O)nc(NC(C)(C)C)n1
Mol. weight [g/mol]: 239.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.47		Crippen Method
logp	1.049		Crippen Method
mcvol	185.340	ml/mol	McGowan Method
rinpol	2002.00		NIST Webbook
rinpol	2002.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373112&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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