(4,6-Dichloro-[1,3,5]triazin-2-yl)-(1,3-dimethyl-buty

Inchi: InChI=1S/C9H14Cl2N4/c1-5(2)4-6(3)12-9-14-7(10)13-8(11)15-9/h5-6H,4H2,1-3H3,(H,12
InchiKey: NBIUQKMFEDVTNB-UHFFFAOYSA-N
Formula: C9H14Cl2N4
SMILES: CC(C)CC(C)Nc1nc(Cl)nc(Cl)n1
Mol. weight [g/mol]: 249.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	3.025		Crippen Method
mcvol	178.310	ml/mol	McGowan Method
rinpol	1702.15		NIST Webbook
rinpol	1731.01		NIST Webbook
rinpol	1702.15		NIST Webbook
rinpol	1711.87		NIST Webbook
rinpol	1731.08		NIST Webbook
rinpol	1731.01		NIST Webbook
rinpol	1740.74		NIST Webbook
rinpol	1702.15		NIST Webbook
rinpol	1731.01		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R288558&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices