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

Inchi: InChI=1S/C9H14Cl2N4/c1-4-5-9(2,3)15-8-13-6(10)12-7(11)14-8/h4-5H2,1-3H3,(H,12,13,
InchiKey: NVWABGIEYVKRIE-UHFFFAOYSA-N
Formula: C9H14Cl2N4
SMILES: CCCC(C)(C)Nc1nc(Cl)nc(Cl)n1
Mol. weight [g/mol]: 249.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Crippen Method
logp	3.169		Crippen Method
mcvol	178.310	ml/mol	McGowan Method
rinpol	1724.43		NIST Webbook
rinpol	1757.99		NIST Webbook
rinpol	1724.43		NIST Webbook
rinpol	1733.69		NIST Webbook
rinpol	1745.10		NIST Webbook
rinpol	1757.99		NIST Webbook
rinpol	1767.29		NIST Webbook
rinpol	1724.43		NIST Webbook
rinpol	1757.99		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R288538&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

rinpol: Non-polar retention indices

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