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

Inchi: InChI=1S/C8H12Cl2N4/c1-4-8(2,3)14-7-12-5(9)11-6(10)13-7/h4H2,1-3H3,(H,11,12,13,14
InchiKey: HIIWFTFAKHZRAW-UHFFFAOYSA-N
Formula: C8H12Cl2N4
SMILES: CCC(C)(C)Nc1nc(Cl)nc(Cl)n1
Mol. weight [g/mol]: 235.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	2.779		Crippen Method
mcvol	164.220	ml/mol	McGowan Method
rinpol	1617.49		NIST Webbook
rinpol	1647.65		NIST Webbook
rinpol	1617.49		NIST Webbook
rinpol	1625.39		NIST Webbook
rinpol	1637.68		NIST Webbook
rinpol	1647.65		NIST Webbook
rinpol	1655.57		NIST Webbook
rinpol	1617.49		NIST Webbook
rinpol	1647.65		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=R288543&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