(4,6-Dichloro-[1,3,5]triazin-2-yl)-(1,1,3-trimethyl-bu

Inchi: InChI=1S/C10H16Cl2N4/c1-6(2)5-10(3,4)16-9-14-7(11)13-8(12)15-9/h6H,5H2,1-4H3,(H,
InchiKey: MVOSQYGIRXHRPQ-UHFFFAOYSA-N
Formula: C10H16Cl2N4
SMILES: CC(C)CC(C)(C)Nc1nc(Cl)nc(Cl)n1
Mol. weight [g/mol]: 263.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	3.415		Crippen Method
mcvol	192.400	ml/mol	McGowan Method
rinpol	1814.45		NIST Webbook
rinpol	1843.66		NIST Webbook
rinpol	1814.45		NIST Webbook
rinpol	1851.85		NIST Webbook
rinpol	1814.45		NIST Webbook
rinpol	1843.66		NIST Webbook
rinpol	1822.63		NIST Webbook
rinpol	1832.88		NIST Webbook
rinpol	1843.66		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=R288523&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