

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

Inchi: InChI=1S/C11H18Cl2N4/c1-10(2,3)6-11(4,5)17-9-15-7(12)14-8(13)16-9/h6H2,1-5H3,(H,1)
InchiKey: HPFWYRKGZUGGPB-UHFFFAOYSA-N
Formula: C11H18Cl2N4
SMILES: CC(C)(C)CC(C)(C)Nc1nc(Cl)nc(Cl)n1
Mol. weight [g/mol]: 277.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.95		Crippen Method
logp	3.805		Crippen Method
mcpvol	206.490	ml/mol	McGowan Method
rinpol	1906.55		NIST Webbook
rinpol	1936.94		NIST Webbook
rinpol	1906.55		NIST Webbook
rinpol	1925.64		NIST Webbook
rinpol	1936.94		NIST Webbook
rinpol	1945.26		NIST Webbook
rinpol	1906.55		NIST Webbook
rinpol	1936.94		NIST Webbook
rinpol	1914.86		NIST Webbook

Sources

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=R288518&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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