(4,6-Dichloro-[1,3,5]triazin-2-yl)-(1-methyl-butyl)-a

Inchi: InChI=1S/C8H12Cl2N4/c1-3-4-5(2)11-8-13-6(9)12-7(10)14-8/h5H,3-4H2,1-2H3,(H,11,12,

InchiKey: RBJAOUBQAQYPIF-UHFFFAOYSA-N

Formula: C8H12Cl2N4

SMILES: CCCC(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	1643.16		NIST Webbook
rinpol	1668.31		NIST Webbook
rinpol	1643.16		NIST Webbook
rinpol	1670.78		NIST Webbook
rinpol	1668.31		NIST Webbook
rinpol	1678.79		NIST Webbook
rinpol	1643.16		NIST Webbook
rinpol	1668.31		NIST Webbook
rinpol	1653.61		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R288563&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