s-Triazine, 2-chloro, 4-(1-methylethyl)amino-6-(1,1-dimethylethyl)amin

Inchi: InChI=1S/C10H18ClN5/c1-6(2)12-8-13-7(11)14-9(15-8)16-10(3,4)5/h6H,1-5H3,(H2,12,13

InchiKey: WHYHGXUTDPTVTE-UHFFFAOYSA-N

Formula: C10H18ClN5

SMILES: CC(C)N=c1nc(Cl)nc(NC(C)(C)C)[nH]1

Mol. weight [g/mol]: 243.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	1.496		Crippen Method
mcvol	190.140	ml/mol	McGowan Method
rinpol	1781.00		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=R104539&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices