6-Chloro-N,N'-(cyclopentyl)-[1,3,5]triazine-2,4-diar

Inchi: InChI=1S/C13H20ClN5/c14-11-17-12(15-9-5-1-2-6-9)19-13(18-11)16-10-7-3-4-8-10/h9-1
InchiKey: GWSSLAIMYRVJSW-UHFFFAOYSA-N
Formula: C13H20ClN5
SMILES: Clc1nc(NC2CCCC2)nc(NC2CCCC2)n1
Mol. weight [g/mol]: 281.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	3.234		Crippen Method
mcvol	210.690	ml/mol	McGowan Method
rinpol	2245.29		NIST Webbook
rinpol	2291.48		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R288489&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.