[1,3,5]Triazine-2,4-diamine, 6-chloro-N,N'-dicycloheptyl-

Inchi: InChI=1S/C17H28ClN5/c18-15-21-16(19-13-9-5-1-2-6-10-13)23-17(22-15)20-14-11-7-3-4-8-12-14/h13-14H,1-12H2,(H2,19,20,21,22,23)

InchiKey: NDHBZABQERFFOL-UHFFFAOYSA-N

Formula: C17H28ClN5

SMILES: Clc1nc(NC2CCCCCC2)nc(NC2CCCCCC2)n1

Mol. weight [g/mol]: 337.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.51		Crippen Method
logp	4.794		Crippen Method
mcvol	267.050	ml/mol	McGowan Method
rinpol	2439.67		NIST Webbook
rinpol	2484.55		NIST Webbook
rinpol	2439.67		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U310215&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices