

[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
InchiKey: NDHBZABQERFFOL-UHFFFAOYSA-N
Formula: C17H28ClN5
SMILES: Clc1nc(NC2CCCCC2)nc(NC2CCCCC2)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

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