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

Inchi: InChI=1S/C11H16ClN5/c12-9-15-10(13-7-3-1-4-7)17-11(16-9)14-8-5-2-6-8/h7-8H,1-6H2,
InchiKey: WGWFUVPOZDRVAO-UHFFFAOYSA-N
Formula: C11H16ClN5
SMILES: Clc1nc(=NC2CCC2)[nH]c(=NC2CCC2)[nH]1
Mol. weight [g/mol]: 253.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	0.334		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
rinpol	2146.08		NIST Webbook
rinpol	2146.08		NIST Webbook
rinpol	2192.25		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R288414&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices