1,3,4,6-Tetrachloro-3alpha,6alpha-diphenyl-glycol

Inchi: InChI=1S/C16H10Cl4N4O2/c17-21-13(25)23(19)16(12-9-5-2-6-10-12)15(21,11-7-3-1-4-8
InchiKey: FJQZXCPWAGYPSD-UHFFFAOYSA-N
Formula: C16H10Cl4N4O2
SMILES: O=C1N(Cl)C2(c3ccccc3)N(Cl)C(=O)N(Cl)C2(c2ccccc2)N1Cl
Mol. weight [g/mol]: 432.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.20		Crippen Method
logp	4.783		Crippen Method
mcvol	259.080	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002584&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