Chlorhexidine

Other names:	1,1'-hexamethylenebis(5-(p-chlorophenyl)biguanide)
	N,N''-bis(4-chlorophenyl)-3,12-diimino-2,4,11,13-tetraazatetradecanediimidamide
	N1,N14-bis(4-chlorophenyl)-3,12-diimino-2,4,11,13-tetraazatetradecanediimidamide
Inchi:	InChI=1S/C22H30Cl2N10/c23-15-5-9-17(10-6-15)31-21(27)33-19(25)29-13-3-1-2-4-14-3
InchiKey:	GHXZTYHSJHQHIJ-UHFFFAOYSA-N
Formula:	C22H30Cl2N10
SMILES:	NC(=NCCCCCCN=C(N)N=C(N)Nc1ccc(Cl)cc1)N=C(N)Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	505.46

Physical Properties

Property code	Value	Unit	Source
logp	3.337		Crippen Method
mcvol	380.400	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Equilibrium solubility, solvent effect and preferential solvation of chlorhexidine in aqueous co-solvent solutions of (methanol, ethanol, N,N-dimethylformamide and 1,4-dioxane):	https://www.doi.org/10.1016/j.jct.2018.09.008
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:
https://www.chemeo.com/cid/101-588-7/Chlorhexidine.pdf