

Chlorthalidone Me

Inchi: InChI=1S/C17H17ClN2O4S/c1-19(2)25(23,24)15-9-8-11(10-14(15)18)17(22)13-7-5-4-6-1
InchiKey: HLNOUGNOJXXPLF-UHFFFAOYSA-N
Formula: C17H17ClN2O4S
SMILES: CN1C(=O)c2ccccc2C1(O)c1ccc(S(=O)(=O)N(C)C)c(Cl)c1
Mol. weight [g/mol]: 380.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	1.869		Crippen Method
mcvol	259.740	ml/mol	McGowan Method
rinpole	2883.00		NIST Webbook
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Sources

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=R39963&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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<https://www.chemeo.com/cid/64-115-3/Chlorthalidone-Me.pdf>

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