1-[[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolan-2-

Inchi: InChI=1S/C15H17Cl2N3O2/c1-2-3-12-7-21-15(22-12,8-20-10-18-9-19-20)13-5-4-11(16)6

InchiKey: STJLVHWMYQXCPB-UHFFFAOYSA-N

Formula: C15H17Cl2N3O2

SMILES: CCCC1COC(Cn2cncn2)(c2ccc(Cl)cc2Cl)O1

Mol. weight [g/mol]: 342.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Aqueous Solubility Prediction Method
logp	3.653		Crippen Method
mcvol	234.290	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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume