Furosemide tetra-methyl derivative

Other names: Furosemide Me, #2
Inchi: InChI=1S/C16H19ClN2O5S/c1-18(2)25(21,22)15-8-12(16(20)23-4)14(9-13(15)17)19(3)1
InchiKey: MRRJJFRJZYQHSF-UHFFFAOYSA-N
Formula: C16H19ClN2O5S
SMILES: COC(=O)c1cc(S(=O)(=O)N(C)C)c(Cl)cc1N(C)Cc1ccco1
Mol. weight [g/mol]: 386.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.82		Crippen Method
logp	2.606		Crippen Method
mcvol	266.680	ml/mol	McGowan Method
rinpol	2742.00		NIST Webbook
rinpol	2742.00		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=U137052&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