

# Furosemide tri-methyl derivative

<b>Other names:</b>	Furosemide, trimethyl
<b>Inchi:</b>	InChI=1S/C15H17ClN2O5S/c1-17-24(20,21)14-7-11(15(19)22-3)13(8-12(14)16)18(2)9-1
<b>InchiKey:</b>	OBJFIKVSHHYZPK-UHFFFAOYSA-N
<b>Formula:</b>	C15H17ClN2O5S
<b>SMILES:</b>	<chem>CNS(=O)(=O)c1cc(C(=O)OC)c(N(C)Cc2ccco2)cc1Cl</chem>
<b>Mol. weight [g/mol]:</b>	372.82

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.02		Crippen Method
logp	2.264		Crippen Method
mcvol	252.590	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U137053&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U137053&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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