

Piretanide + TMAH

Other names:	Piretanide, trimethyl deriv.
Inchi:	InChI=1S/C20H24N2O5S/c1-21(2)28(24,25)18-14-15(20(23)26-3)13-17(22-11-7-8-12-22)
InchiKey:	JLYNDJGRHUBDOF-UHFFFAOYSA-N
Formula:	C20H24N2O5S
SMILES:	<chem>COC(=O)c1cc(N2CCCC2)c(Oc2ccccc2)c(S(=O)(=O)N(C)C)c1</chem>
Mol. weight [g/mol]:	404.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Crippen Method
logp	3.116		Crippen Method
mcvol	295.640	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U74688&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/96-433-5/Piretanide-TMAH.pdf>

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