

# P-toluenesulfonamide], n,n'-dithiodiethylenebis[n-(2-thenyl)-

<b>Inchi:</b>	InChI=1S/C28H32N2O4S6/c1-23-7-11-27(12-8-23)39(31,32)29(21-25-5-3-17-35-25)15-1
<b>InchiKey:</b>	LMWRCROKJGBKBO-UHFFFAOYSA-N
<b>Formula:</b>	C28H32N2O4S6
<b>SMILES:</b>	Cc1ccc(S(=O)(=O)N(CCSSCCN(Cc2cccs2)S(=O)(=O)c2ccc(C)cc2)Cc2cccs2)cc1
<b>Mol. weight [g/mol]:</b>	652.96
<b>CAS:</b>	103458-90-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.75		Crippen Method
logp	6.890		Crippen Method
mcvol	460.480	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C103458908&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C103458908&amp;Units=SI</a>
<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>

## 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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