

# 3,6-Dimethoxy-4,5-epoxyphenanthrene

<b>Inchi:</b>	InChI=1S/C16H12O3/c1-17-11-7-5-9-3-4-10-6-8-12(18-2)16-14(10)13(9)15(11)19-16/h3-
<b>InchiKey:</b>	YHUFSDUFQNMKL-UHFFFAOYSA-N
<b>Formula:</b>	C16H12O3
<b>SMILES:</b>	COc1ccc2ccc3ccc(OC)c4oc1c2c34
<b>Mol. weight [g/mol]:</b>	252.26

## Physical Properties

Property code	Value	Unit	Source
log10ws	-10.27		Crippen Method
logp	4.194		Crippen Method
mcvol	180.370	ml/mol	McGowan Method
rinpola	2333.00		NIST Webbook
rinpola	2333.00		NIST Webbook

## 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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R330748&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R330748&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
<b>rinpola:</b>	Non-polar retention indices

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