

# 9H-Thioxanthen-9-one, 2-(1-methylethyl)-

<b>Other names:</b>	2-(1-methylethyl)-9H-thioxanthen-9-one 2-isopropyl-9H-thioxanthen-9-one 2-isopropylthioxanthone 9H-Thioxanthen-9-one, 2-isopropyl Quantacure ITX Quantacure ITX (Isopropylthioxanthene-9-one)
<b>Inchi:</b>	InChI=1S/C16H14OS/c1-10(2)11-7-8-15-13(9-11)16(17)12-5-3-4-6-14(12)18-15/h3-10H,
<b>InchiKey:</b>	KTALPKYXQZGAEG-UHFFFAOYSA-N
<b>Formula:</b>	C16H14OS
<b>SMILES:</b>	CC(C)c1ccc2sc3ccccc3c(=O)c2c1
<b>Mol. weight [g/mol]:</b>	254.35
<b>CAS:</b>	5495-84-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	4.538		Crippen Method
mcpvol	195.840	ml/mol	McGowan Method
rinpol	2345.00		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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Determination and Correlation of Solubilities of 2-Isopropylthioxanthone in Several Different Solvents from (299.15 to 329.85) K:</b>	<a href="https://www.doi.org/10.1021/je501011t">https://www.doi.org/10.1021/je501011t</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=C5495841&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5495841&amp;Units=SI</a>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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