

# 3(2H)-Isothiazolone, 2-octyl-

<b>Other names:</b>	4-Isothiazolin-3-one, 2-octyl- Kathon LP Preservative Octyl-4-isothiazol-3-one Skane M 8 2-n-Octyl-3-isothiazolone 2-n-Octyl-4-isothiazolin-3-one 2-Octyl-3-isothiazolinone 2-Octyl-3-isothiazolone 2-Octyl-3-isothioazolone 2-Octyl-3(2H)-isothiazolone 2-Octyl-4-isothiazolin-3-one Kathon 893 Kathon sp 70 Micro-Chek 11 Micro-chek 11D Micro-chek skane Microbicide M-8 Othilinone Octyl-3(2H)-isothiazolone Pancil Pancil T RH-893 Skane 8 Kathon 4200 Kathon 893F Kathon LM Vinyzene IT 3000DIDP 2-octyl-2H-isothiazol-3-one
<b>Inchi:</b>	InChI=1S/C11H19NOS/c1-2-3-4-5-6-7-9-12-11(13)8-10-14-12/h8,10H,2-7,9H2,1H3
<b>InchiKey:</b>	JPMIIZHYWMDT-UHFFFAOYSA-N
<b>Formula:</b>	C11H19NOS
<b>SMILES:</b>	CCCCCCCn1sccc1=O
<b>Mol. weight [g/mol]:</b>	213.34
<b>CAS:</b>	26530-20-1

## Physical Properties

Property code	Value	Unit	Source
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log10ws	-3.42		Crippen Method
logp	3.270		Crippen Method
mcvol	178.590	ml/mol	McGowan Method
rinsol	1849.00		NIST Webbook
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## Sources

<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=C26530201&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C26530201&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>

## 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>rinsol:</b>	Non-polar retention indices

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