

# 2-Nonylidene-1,3-dithiolane

<b>Inchi:</b>	InChI=1S/C12H22S2/c1-2-3-4-5-6-7-8-9-12-13-10-11-14-12/h9H,2-8,10-11H2,1H3
<b>InchiKey:</b>	QTRGCABSLUYSHT-UHFFFAOYSA-N
<b>Formula:</b>	C12H22S2
<b>SMILES:</b>	CCCCCCCCC=C1SCCS1
<b>Mol. weight [g/mol]:</b>	230.43

## Physical Properties

Property code	Value	Unit	Source
gf	219.60	kJ/mol	Joback Method
hf	-43.64	kJ/mol	Joback Method
hfus	27.34	kJ/mol	Joback Method
hvap	55.28	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	5.058		Crippen Method
mcvol	197.480	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
tb	596.21	K	Joback Method
tc	810.59	K	Joback Method
tf	417.40	K	Joback Method
vc	0.725	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.04	J/mol×K	596.21	Joback Method
cpg	500.75	J/mol×K	631.94	Joback Method
cpg	517.42	J/mol×K	667.67	Joback Method
cpg	533.12	J/mol×K	703.40	Joback Method
cpg	547.91	J/mol×K	739.13	Joback Method
cpg	561.83	J/mol×K	774.86	Joback Method
cpg	574.97	J/mol×K	810.59	Joback Method

# 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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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=R391134&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R391134&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<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>pc:</b>	Critical Pressure
<b>rinp:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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