

# 3-Nonanone, 2,4-chloro (RR, SS)

Inchi:	InChI=1S/C9H16Cl2O/c1-3-4-5-6-8(11)9(12)7(2)10/h7-8H,3-6H2,1-2H3
InchiKey:	NYJAYMSCABMYSY-UHFFFAOYSA-N
Formula:	C9H16Cl2O
SMILES:	CCCCC(Cl)C(=O)C(C)Cl
Mol. weight [g/mol]:	211.13

## Physical Properties

Property code	Value	Unit	Source
gf	-132.76	kJ/mol	Joback Method
hf	-383.71	kJ/mol	Joback Method
hfus	22.01	kJ/mol	Joback Method
hvap	50.37	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.370		Crippen Method
mvol	163.720	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1308.00		NIST Webbook
rinpol	1308.00		NIST Webbook
tb	533.17	K	Joback Method
tc	725.90	K	Joback Method
tf	270.96	K	Joback Method
vc	0.631	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.23	J/molxK	533.17	Joback Method
cpg	369.31	J/molxK	565.29	Joback Method
cpg	381.74	J/molxK	597.41	Joback Method
cpg	393.53	J/molxK	629.54	Joback Method
cpg	404.71	J/molxK	661.66	Joback Method
cpg	415.29	J/molxK	693.78	Joback Method
cpg	425.29	J/molxK	725.90	Joback Method
dvisc	0.0069990	Paxs	270.96	Joback Method

dvisc	0.0027503	Paxs	314.66	Joback Method
dvisc	0.0013572	Paxs	358.36	Joback Method
dvisc	0.0007809	Paxs	402.07	Joback Method
dvisc	0.0005008	Paxs	445.77	Joback Method
dvisc	0.0003476	Paxs	489.47	Joback Method
dvisc	0.0002562	Paxs	533.17	Joback Method

## Sources

<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=R630276&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R630276&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>hvap:</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>rinpol:</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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