

# 4,5-epoxy-2-nonenal

Inchi:	InChI=1S/C9H16O2/c1-2-3-5-8-9(11-8)6-4-7-10/h7-9H,2-6H2,1H3
InchiKey:	HDVFGBUZSPCZQT-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	CCCCC1OC1CCC=O
Mol. weight [g/mol]:	156.22

## Physical Properties

Property code	Value	Unit	Source
gf	-107.70	kJ/mol	Joback Method
hf	-394.21	kJ/mol	Joback Method
hfus	28.54	kJ/mol	Joback Method
hvap	46.46	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.923		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
ripol	1875.00		NIST Webbook
tb	483.00	K	Joback Method
tc	665.54	K	Joback Method
tf	273.46	K	Joback Method
vc	0.533	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.62	J/molxK	483.00	Joback Method
cpg	329.72	J/molxK	513.42	Joback Method
cpg	343.14	J/molxK	543.85	Joback Method
cpg	355.90	J/molxK	574.27	Joback Method
cpg	368.04	J/molxK	604.70	Joback Method
cpg	379.56	J/molxK	635.12	Joback Method
cpg	390.52	J/molxK	665.54	Joback Method
dvisc	0.0023518	Paxs	273.46	Joback Method
dvisc	0.0016789	Paxs	308.38	Joback Method

dvisc	0.0012836	Paxs	343.31	Joback Method
dvisc	0.0010313	Paxs	378.23	Joback Method
dvisc	0.0008598	Paxs	413.15	Joback Method
dvisc	0.0007374	Paxs	448.08	Joback Method
dvisc	0.0006466	Paxs	483.00	Joback Method

## 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>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=R325672&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R325672&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>

## 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>ripol:</b>	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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