

# Formic acid, oct-2-yl ester

<b>Inchi:</b>	InChI=1S/C9H18O2/c1-3-4-5-6-7-9(2)11-8-10/h8-9H,3-7H2,1-2H3
<b>InchiKey:</b>	CQRBMEAOKCDBEA-UHFFFAOYSA-N
<b>Formula:</b>	C9H18O2
<b>SMILES:</b>	CCCCCCC(C)OC=O
<b>Mol. weight [g/mol]:</b>	158.24

## Physical Properties

Property code	Value	Unit	Source
gf	-182.06	kJ/mol	Joback Method
hf	-452.17	kJ/mol	Joback Method
hfus	19.02	kJ/mol	Joback Method
hvap	44.37	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.518		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinsol	1083.00		NIST Webbook
tb	475.96	K	Joback Method
tc	648.93	K	Joback Method
tf	240.42	K	Joback Method
vc	0.569	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.93	J/mol×K	475.96	Joback Method
cpg	337.17	J/mol×K	504.79	Joback Method
cpg	349.94	J/mol×K	533.62	Joback Method
cpg	362.22	J/mol×K	562.44	Joback Method
cpg	374.02	J/mol×K	591.27	Joback Method
cpg	385.36	J/mol×K	620.10	Joback Method
cpg	396.23	J/mol×K	648.93	Joback Method
dvisc	0.0055140	Paxs	240.42	Joback Method
dvisc	0.0022829	Paxs	279.68	Joback Method

dvisc	0.0011744	Paxs	318.93	Joback Method
dvisc	0.0006989	Paxs	358.19	Joback Method
dvisc	0.0004608	Paxs	397.45	Joback Method
dvisc	0.0003274	Paxs	436.70	Joback Method
dvisc	0.0002462	Paxs	475.96	Joback Method

## Sources

<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=U368945&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368945&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>
<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>

## 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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