

# Formic acid, hept-3-yl ester

<b>Inchi:</b>	InChI=1S/C8H16O2/c1-3-5-6-8(4-2)10-7-9/h7-8H,3-6H2,1-2H3
<b>InchiKey:</b>	RJJVYSJFEOFICB-UHFFFAOYSA-N
<b>Formula:</b>	C8H16O2
<b>SMILES:</b>	CCCCC(CC)OC=O
<b>Mol. weight [g/mol]:</b>	144.21

## Physical Properties

Property code	Value	Unit	Source
gf	-190.48	kJ/mol	Joback Method
hf	-431.53	kJ/mol	Joback Method
hfus	16.43	kJ/mol	Joback Method
hvap	42.14	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.128		Crippen Method
mvol	131.020	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	982.00		NIST Webbook
rinpol	982.00		NIST Webbook
tb	453.08	K	Joback Method
tc	627.37	K	Joback Method
tf	229.15	K	Joback Method
vc	0.512	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.99	J/mol×K	453.08	Joback Method
cpg	293.22	J/mol×K	482.13	Joback Method
cpg	305.02	J/mol×K	511.18	Joback Method
cpg	316.38	J/mol×K	540.23	Joback Method
cpg	327.32	J/mol×K	569.27	Joback Method
cpg	337.83	J/mol×K	598.32	Joback Method
cpg	347.93	J/mol×K	627.37	Joback Method
dvisc	0.0055375	Paxs	229.15	Joback Method

dvisc	0.0023301	Paxs	266.47	Joback Method
dvisc	0.0012128	Paxs	303.79	Joback Method
dvisc	0.0007283	Paxs	341.12	Joback Method
dvisc	0.0004836	Paxs	378.44	Joback Method
dvisc	0.0003456	Paxs	415.76	Joback Method
dvisc	0.0002610	Paxs	453.08	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U368765&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368765&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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