

# Hexanal dimethyl acetal

<b>Other names:</b>	Hexane, 1,1-dimethoxy- 1,1-Dimethoxyhexane
<b>Inchi:</b>	InChI=1S/C8H18O2/c1-4-5-6-7-8(9-2)10-3/h8H,4-7H2,1-3H3
<b>InchiKey:</b>	ZQUJUCJLDXTKKW-UHFFFAOYSA-N
<b>Formula:</b>	C8H18O2
<b>SMILES:</b>	CCCCCC(OC)OC
<b>Mol. weight [g/mol]:</b>	146.23
<b>CAS:</b>	1599-47-9

## Physical Properties

Property code	Value	Unit	Source
gf	-195.96	kJ/mol	Joback Method
hf	-478.17	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	37.83	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.186		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	929.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	964.00		NIST Webbook
ripol	1156.00		NIST Webbook
tb	426.84	K	Joback Method
tc	594.62	K	Joback Method
tf	209.38	K	Joback Method
vc	0.513	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.43	J/molxK	426.84	Joback Method
cpg	295.24	J/molxK	454.80	Joback Method
cpg	307.70	J/molxK	482.77	Joback Method

cpg	319.80	J/molxK	510.73	Joback Method
cpg	331.54	J/molxK	538.70	Joback Method
cpg	342.91	J/molxK	566.66	Joback Method
cpg	353.90	J/molxK	594.62	Joback Method
dvisc	0.0048555	Paxs	209.38	Joback Method
dvisc	0.0018809	Paxs	245.62	Joback Method
dvisc	0.0009298	Paxs	281.87	Joback Method
dvisc	0.0005397	Paxs	318.11	Joback Method
dvisc	0.0003502	Paxs	354.35	Joback Method
dvisc	0.0002462	Paxs	390.60	Joback Method
dvisc	0.0001837	Paxs	426.84	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=C1599479&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1599479&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>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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