

# [2,3-2H2]-(E)-2-Octenal

Inchi:	InChI=1S/C8H14O/c1-2-3-4-5-6-7-8-9/h6-8H,2-5H2,1H3/b7-6+/i6D,7D
InchiKey:	LVBXEMGDVWVTGY-ITRJFYCISA-N
Formula:	C8H12D2O
SMILES:	CCCCC=CC=O
Mol. weight [g/mol]:	128.21

## Physical Properties

Property code	Value	Unit	Source
gf	-2.82	kJ/mol	Joback Method
hf	-176.81	kJ/mol	Joback Method
hfus	18.97	kJ/mol	Joback Method
hvap	40.08	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
ripol	1059.00		NIST Webbook
ripol	1059.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1424.00		NIST Webbook
tb	435.26	K	Joback Method
tc	614.34	K	Joback Method
tf	216.84	K	Joback Method
vc	0.480	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.07	J/molxK	435.26	Joback Method
cpg	252.93	J/molxK	465.11	Joback Method
cpg	264.25	J/molxK	494.95	Joback Method
cpg	275.03	J/molxK	524.80	Joback Method
cpg	285.31	J/molxK	554.65	Joback Method

cpg	295.10	J/molxK	584.49	Joback Method
cpg	304.43	J/molxK	614.34	Joback Method
dvisc	0.0045537	Paxs	216.84	Joback Method
dvisc	0.0020114	Paxs	253.24	Joback Method
dvisc	0.0010910	Paxs	289.65	Joback Method
dvisc	0.0006784	Paxs	326.05	Joback Method
dvisc	0.0004641	Paxs	362.45	Joback Method
dvisc	0.0003402	Paxs	398.86	Joback Method
dvisc	0.0002628	Paxs	435.26	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R396075&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R396075&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>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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