

# 2-Octenoic acid, (E)-

<b>Other names:</b>	(2E)-2-Octenoic acid 2-Octenoic acid 2-Octenoic acid, trans- 2E-octenoic acid oct-2-enoic acid trans-2-Octenoic acid
<b>Inchi:</b>	InChI=1S/C8H14O2/c1-2-3-4-5-6-7-8(9)10/h6-7H,2-5H2,1H3,(H,9,10)/b7-6+
<b>InchiKey:</b>	CWMPPVPFLSZGCY-VOTSOKGWSA-N
<b>Formula:</b>	C8H14O2
<b>SMILES:</b>	CCCCC=CC(=O)O
<b>Mol. weight [g/mol]:</b>	142.20
<b>CAS:</b>	1871-67-6

## Physical Properties

Property code	Value	Unit	Source
gf	-169.04	kJ/mol	Joback Method
hf	-356.04	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	56.78	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.208		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
rinpol	1245.00		NIST Webbook
rinpol	1245.00		NIST Webbook
ripol	2182.00		NIST Webbook
ripol	2182.00		NIST Webbook
tb	532.65	K	Joback Method
tc	708.47	K	Joback Method
tf	285.59	K	Joback Method
vc	0.488	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.94	J/mol×K	532.65	Joback Method
cpg	301.30	J/mol×K	561.95	Joback Method
cpg	311.18	J/mol×K	591.26	Joback Method
cpg	320.59	J/mol×K	620.56	Joback Method
cpg	329.56	J/mol×K	649.86	Joback Method
cpg	338.09	J/mol×K	679.17	Joback Method
cpg	346.22	J/mol×K	708.47	Joback Method
dvisc	0.0161455	Paxs	285.59	Joback Method
dvisc	0.0042862	Paxs	326.77	Joback Method
dvisc	0.0015311	Paxs	367.94	Joback Method
dvisc	0.0006729	Paxs	409.12	Joback Method
dvisc	0.0003437	Paxs	450.30	Joback Method
dvisc	0.0001965	Paxs	491.47	Joback Method
dvisc	0.0001225	Paxs	532.65	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41450e+01
Coeff. B	-4.25411e+03
Coeff. C	-8.28880e+01
Temperature range (K), min.	389.88
Temperature range (K), max.	564.47

## Sources

The Yaws Handbook of Vapor Pressure:  
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>  
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Joback Method:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1871676&Units=SI>

# 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>pvap:</b>	Vapor pressure
<b>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</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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