2-Octene, (E)-

Other names:	(2E)-2-Octene
	(E)-2-C8H16
	(E)-2-OCTENE
	(E)-Oct-2-ene
	.beta.-trans-octene
	Oct-2(E)-ene
	TRANS-2-OCTENE
	trans-oct-2-ene
Inchi:	InChI=1S/C8H16/c1-3-5-7-8-6-4-2/h3,5H,4,6-8H2,1-2H3/b5-3+
InchiKey:	ILPBINAXDRFYPL-HWKANZROSA-N
Formula:	C8H16
SMILES:	CC=CCCCCC
Mol. weight [g/mol]:	112.21
CAS:	13389-42-9

Physical Properties

Property code	Value	Unit	Source
af	0.3500		KDB
gf	92.74	kJ/mol	KDB
hcg	5315.77	kJ/mol	KDB
hcn	4963.898	kJ/mol	KDB
hf	-94.58	kJ/mol	KDB
hfus	16.68	kJ/mol	Joback Method
hvap	40.20	kJ/mol	NIST Webbook
ie	8.91 ± 0.01	eV	NIST Webbook
ie	9.09 ± 0.01	eV	NIST Webbook
log10ws	-3.02		Crippen Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2770.00	kPa	KDB
rinpol	803.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	798.00		NIST Webbook

rinpol	817.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	818.00	NIST Webbook
rinpol	818.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	809.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	801.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	803.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	797.40	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	799.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	803.00	NIST Webbook
rinpol	803.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	797.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	792.00	NIST Webbook
rinpol	797.50	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	798.20	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	797.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	803.60	NIST Webbook
rinpol	797.20	NIST Webbook
rinpol	797.00	NIST Webbook
rinpol	797.30	NIST Webbook

rinpol	797.70		NIST Webbook
rinpol	799.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	797.90		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	803.00		NIST Webbook
rinpol	805.00		NIST Webbook
ripol	864.00		NIST Webbook
ripol	866.00		NIST Webbook
ripol	853.00		NIST Webbook
ripol	861.00		NIST Webbook
ripol	864.00		NIST Webbook
ripol	854.00		NIST Webbook
ripol	864.00		NIST Webbook
ripol	861.00		NIST Webbook
ripol	852.00		NIST Webbook
ripol	853.00		NIST Webbook
ripol	866.00		NIST Webbook
ripol	866.00		NIST Webbook
ripol	866.50		NIST Webbook
ripol	864.30		NIST Webbook
ripol	865.70		NIST Webbook
ripol	864.00		NIST Webbook
ripol	866.50		NIST Webbook
ripol	864.00		NIST Webbook
ripol	864.30		NIST Webbook
ripol	865.70		NIST Webbook
ripol	866.00		NIST Webbook
ripol	864.00		NIST Webbook
ripol	865.70		NIST Webbook
ripol	860.00		NIST Webbook
tb	398.26 ± 0.20	K	NIST Webbook
tb	398.09 ± 0.30	K	NIST Webbook
tb	398.35 ± 0.50	K	NIST Webbook
tb	397.40 ± 0.60	K	NIST Webbook
tb	397.40 ± 0.60	K	NIST Webbook
tb	398.10	K	KDB
tb	396.20	K	NIST Webbook
tb	398.09 ± 0.30	K	NIST Webbook
tb	398.20	K	NIST Webbook
tb	396.00	K	NIST Webbook
tb	396.50 ± 1.00	K	NIST Webbook

tc	580.00	K	KDB
tc	569.80	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	185.15 ± 1.50	K	NIST Webbook
tf	185.40	K	KDB
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.62	J/mol×K	558.45	Joback Method
cpg	218.05	J/mol×K	386.60	Joback Method
cpg	230.94	J/mol×K	415.24	Joback Method
cpg	243.29	J/mol×K	443.88	Joback Method
cpg	255.11	J/mol×K	472.53	Joback Method
cpg	266.43	J/mol×K	501.17	Joback Method
cpg	277.26	J/mol×K	529.81	Joback Method
dvisc	0.0002015	Pa×s	386.60	Joback Method
dvisc	0.0052396	Pa×s	174.84	Joback Method
dvisc	0.0019294	Pa×s	210.13	Joback Method
dvisc	0.0009470	Pa×s	245.43	Joback Method
dvisc	0.0005559	Pa×s	280.72	Joback Method
dvisc	0.0003675	Pa×s	316.01	Joback Method
dvisc	0.0002641	Pa×s	351.31	Joback Method
hvapt	37.90	kJ/mol	377.50	NIST Webbook
rfi	1.41070		298.15	KDB
rhol	720.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47525e+01
Coeff. B	-3.56590e+03
Coeff. C	-4.14850e+01
Temperature range (K), min.	288.01

Temperature range (K), max.	419.19

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.58492e+01
Coeff. B	-6.79412e+03
Coeff. C	-7.48209e+00
Coeff. D	3.98341e-06
Temperature range (K), min.	185.45
Temperature range (K), max.	577.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=251
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=251
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13389429&Units=SI
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume