4-Octene, (E)-

Other names:	(4E)-4-Octene
	(E)-4-C8H16
	(E)-4-OCTENE
	(E)-Oct-4-ene
	TRANS-4-OCTENE
	n-trans-4-Octene
	trans-n-4-Octene
	trans-oct-4-ene
Inchi:	InChI=1S/C8H16/c1-3-5-7-8-6-4-2/h7-8H,3-6H2,1-2H3/b8-7+
InchiKey:	IRUCBBFNLDIMIK-BQYQJAHWSA-N
Formula:	C8H16
SMILES:	CCCC=CCCC
Mol. weight [g/mol]:	112.21
CAS:	14850-23-8

Physical Properties

Property code	Value	Unit	Source
gf	96.70	kJ/mol	Joback Method
hf	-91.23	kJ/mol	Joback Method
hfus	16.68	kJ/mol	Joback Method
hvap	42.90 ± 0.30	kJ/mol	NIST Webbook
hvap	39.70	kJ/mol	NIST Webbook
ie	8.83 ± 0.01	eV	NIST Webbook
ie	9.01 ± 0.01	eV	NIST Webbook
ie	8.84 ± 0.01	eV	NIST Webbook
log10ws	-3.02		Crippen Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	782.90		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	792.80		NIST Webbook
rinpol	793.10		NIST Webbook
rinpol	783.90		NIST Webbook
rinpol	784.10		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	795.00		NIST Webbook

rinpol	795.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	786.50	NIST Webbook
rinpol	786.50	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	784.40	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	786.90	NIST Webbook
rinpol	783.40	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	784.10	NIST Webbook
rinpol	784.20	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	794.25	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	797.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	802.00	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	794.25	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	797.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	794.70	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	784.60	NIST Webbook
ripol	840.00	NIST Webbook

ripol	841.00		NIST Webbook
ripol	839.00		NIST Webbook
ripol	839.00		NIST Webbook
ripol	842.00		NIST Webbook
ripol	840.10		NIST Webbook
ripol	839.30		NIST Webbook
ripol	839.00		NIST Webbook
ripol	841.90		NIST Webbook
ripol	839.00		NIST Webbook
ripol	840.10		NIST Webbook
ripol	839.30		NIST Webbook
ripol	841.90		NIST Webbook
ripol	841.00		NIST Webbook
ripol	841.00		NIST Webbook
tb	395.50	K	NIST Webbook
tb	393.85 ± 1.50	K	NIST Webbook
tb	395.52 ± 0.20	K	NIST Webbook
tb	397.00	K	NIST Webbook
tb	393.40 ± 2.00	K	NIST Webbook
tb	395.50 ± 0.20	K	NIST Webbook
tb	395.38 ± 0.30	K	NIST Webbook
tb	395.55 ± 0.50	K	NIST Webbook
tb	395.25 ± 0.60	K	NIST Webbook
tb	395.44 ± 0.30	K	NIST Webbook
tb	395.44 ± 0.30	K	NIST Webbook
tb	395.52 ± 0.20	K	NIST Webbook
tb	395.44 ± 0.30	K	NIST Webbook
tc	566.30	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	174.84	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.26	J/mol×K	529.81	Joback Method
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
dvisc	0.0002015	Pa×s	386.60	Joback Method
dvisc	0.0002641	Pa×s	351.31	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
hvapt	37.40	kJ/mol	374.50	NIST Webbook
hvapt	43.20 ± 0.30	kJ/mol	292.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.20	K	98.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42776e+01
Coeff. B	-3.37979e+03
Coeff. C	-4.51000e+01
Temperature range (K), min.	286.69
Temperature range (K), max.	422.05

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.85573e+01
Coeff. B	-7.30681e+03
Coeff. C	-9.42308e+00
Coeff. D	5.67786e-06
Temperature range (K), min.	179.37
Temperature range (K), max.	573.00

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=255
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=255
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14850238&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
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume