3-Octene, (E)-

Other names:	(3E)-3-Octene
	(E)-3-C8H16
	(E)-3-OCTENE
	(E)-Oct-3-ene
	TRANS-3-OCTENE
Inchi:	InChI=1S/C8H16/c1-3-5-7-8-6-4-2/h5,7H,3-4,6,8H2,1-2H3/b7-5+
InchiKey:	YCTDZYMMFQCTEO-FNORWQNLSA-N
Formula:	C8H16
SMILES:	CCC=CCCCC
Mol. weight [g/mol]:	112.21
CAS:	14919-01-8

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	40.20	kJ/mol	NIST Webbook
ie	9.03 ± 0.01	eV	NIST Webbook
ie	8.85 ± 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	796.35		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	797.00		NIST Webbook
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rinpol	794.00		NIST Webbook

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rinpol	788.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	791.50	NIST Webbook
rinpol	788.50	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	788.40	NIST Webbook
rinpol	790.00	NIST Webbook
rinpol	796.35	NIST Webbook
rinpol	814.30	NIST Webbook
rinpol	797.00	NIST Webbook
rinpol	797.00	NIST Webbook
rinpol	797.70	NIST Webbook
rinpol	796.00	NIST Webbook
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rinpol	797.70	NIST Webbook
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rinpol	789.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	814.30	NIST Webbook
rinpol	797.00	NIST Webbook
ripol	847.30	NIST Webbook
ripol	851.30	NIST Webbook
ripol	851.00	NIST Webbook
ripol	851.00	NIST Webbook
ripol	852.00	NIST Webbook
ripol	847.00	NIST Webbook
ripol	847.00	NIST Webbook
ripol	850.00	NIST Webbook
ripol	851.30	NIST Webbook
ripol	847.30	NIST Webbook
ripol	847.20	NIST Webbook

ripol	849.90		NIST Webbook
ripol	847.20		NIST Webbook
ripol	851.30		NIST Webbook
ripol	849.90		NIST Webbook
tb	386.60	K	Joback Method
tc	558.45	K	Joback Method
tf	165.15 ± 1.50	K	NIST Webbook
tf	166.00 ± 2.00	K	NIST Webbook
tf	163.15 ± 0.20	K	NIST Webbook
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	37.60	kJ/mol	375.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43634e+01
Coeff. B	-3.47660e+03
Coeff. C	-3.96640e+01

Temperature range (K), min.	286.66
Temperature range (K), max.	423.74

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.82395e+01
Coeff. B	-6.88658e+03
Coeff. C	-7.84335e+00
Coeff. D	4.27479e-06
Temperature range (K), min.	163.15
Temperature range (K), max.	574.00

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=253

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14919018&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=253

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume