2-Octene

Other names:	2-Octene (mixed cis, trans isomers)
	Oct-2-ene
	Octene-2
Inchi:	InChI=1S/C8H16/c1-3-5-7-8-6-4-2/h3,5H,4,6-8H2,1-2H3
InchiKey:	ILPBINAXDRFYPL-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CC=CCCCCC
Mol. weight [g/mol]:	112.21
CAS:	111-67-1

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	33.36	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	815.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	804.40		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	799.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	802.50		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	804.40		NIST Webbook

rinpol	805.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	813.00		NIST Webbook
ripol	843.00		NIST Webbook
ripol	875.00		NIST Webbook
ripol	880.00		NIST Webbook
ripol	846.00		NIST Webbook
ripol	843.00		NIST Webbook
ripol	864.00		NIST Webbook
ripol	846.00		NIST Webbook
ripol	842.00		NIST Webbook
ripol	848.00		NIST Webbook
ripol	854.00		NIST Webbook
ripol	850.00		NIST Webbook
ripol	858.00		NIST Webbook
ripol	843.00		NIST Webbook
ripol	860.00		NIST Webbook
tb	398.20 ± 1.50	K	NIST Webbook
tb	398.65 ± 3.00	K	NIST Webbook
tb	398.25 ± 0.30	K	NIST Webbook
tb	398.30 ± 0.20	K	NIST Webbook
tb	396.40 ± 3.00	K	NIST Webbook
tb	397.35 ± 2.00	K	NIST Webbook
tb	398.35 ± 0.50	K	NIST Webbook
tb	398.35 ± 0.60	K	NIST Webbook
tb	398.30 ± 0.60	K	NIST Webbook
tb	398.35 ± 0.70	K	NIST Webbook
tb	398.15 ± 2.00	K	NIST Webbook
tb	398.15 ± 2.00	K	NIST Webbook
tb	397.15 ± 4.00	K	NIST Webbook
tb	397.40 ± 0.40	K	NIST Webbook
tb	398.35 ± 0.30	K	NIST Webbook
tb	397.40 ± 0.50	K	NIST Webbook
tc	558.45	K	Joback Method
tf	179.11 ± 0.30	K	NIST Webbook
tf	179.11 ± 0.20	K	NIST Webbook
tf	179.00 ± 2.00	K	NIST Webbook
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	287.62	J/mol×K	558.45	Joback Method
cpl	239.30	J/mol×K	298.00	NIST Webbook
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
dvisc	0.0002015	Pa×s	386.60	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49776e+01
Coeff. B	-3.58631e+03
Coeff. C	-5.18080e+01
Temperature range (K), min.	295.94
Temperature range (K), max.	422.82

Sources

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

Chemical Equilibrium of the Liquid-Phase Dehydration of 1-Octanol to 1-(Octyloxy)octane: https://www.doi.org/10.1021/je301236k

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=C111671&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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