

4-Octene, (Z)-

Other names:	(4Z)-4-Octene (Z)-4-C ₈ H ₁₆ (Z)-4-OCTENE (Z)-Oct-4-ene CIS-4-OCTENE
Inchi:	InChI=1S/C ₈ H ₁₆ /c1-3-5-7-8-6-4-2/h7-8H,3-6H ₂ ,1-2H ₃ /b8-7-
InchiKey:	IRUCBBFNLDIMIK-FPLPWBNLSA-N
Formula:	C ₈ H ₁₆
SMILES:	CCCC=CCCC
Mol. weight [g/mol]:	112.21
CAS:	7642-15-1

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	39.70	kJ/mol	NIST Webbook
ie	8.84 ± 0.01	eV	NIST Webbook
ie	9.03 ± 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	798.00		NIST Webbook
rinpol	789.50		NIST Webbook
rinpol	788.70		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	794.30		NIST Webbook
rinpol	789.50		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	788.60		NIST Webbook
rinpol	787.90		NIST Webbook
rinpol	786.00		NIST Webbook

rinpol	806.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	799.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	799.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	799.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	785.30		NIST Webbook
rinpol	798.50		NIST Webbook
rinpol	799.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	787.90		NIST Webbook
ripol	852.70		NIST Webbook
ripol	857.00		NIST Webbook
ripol	856.60		NIST Webbook
ripol	851.90		NIST Webbook
ripol	852.70		NIST Webbook
ripol	851.90		NIST Webbook
ripol	857.00		NIST Webbook
ripol	858.00		NIST Webbook
ripol	852.00		NIST Webbook
ripol	853.00		NIST Webbook
ripol	854.00		NIST Webbook
ripol	851.90		NIST Webbook
ripol	856.60		NIST Webbook
ripol	856.60		NIST Webbook
tb	395.69 ± 0.30	K	NIST Webbook
tb	395.70	K	NIST Webbook
tb	395.67 ± 0.50	K	NIST Webbook

tb	395.82 ± 0.20	K	NIST Webbook
tb	393.40 ± 0.40	K	NIST Webbook
tc	558.45	K	Joback Method
tf	154.13 ± 0.50	K	NIST Webbook
tf	155.00 ± 2.00	K	NIST Webbook
tf	155.15 ± 1.50	K	NIST Webbook
tf	153.83 ± 1.00	K	NIST Webbook
tf	154.45 ± 0.20	K	NIST Webbook
vc	0.464	m ³ /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	Paxs	386.60	Joback Method
dvisc	0.0052396	Paxs	174.84	Joback Method
dvisc	0.0019294	Paxs	210.13	Joback Method
dvisc	0.0009470	Paxs	245.43	Joback Method
dvisc	0.0005559	Paxs	280.72	Joback Method
dvisc	0.0003675	Paxs	316.01	Joback Method
dvisc	0.0002641	Paxs	351.31	Joback Method
hvapt	37.20	kJ/mol	374.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42712e+01
Coeff. B	-3.29113e+03
Coeff. C	-5.47510e+01
Temperature range (K), min.	290.11

Temperature range (K), max.	422.08
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Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.48977e+01
Coeff. B	-7.89801e+03
Coeff. C	-1.19967e+01
Coeff. D	9.12282e-06
Temperature range (K), min.	288.15
Temperature range (K), max.	423.15

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=254
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=254
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7642151&Units=SI

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

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