Octane, 3-methyl-

Other names:	3-Methyloctane
	Isononane
Inchi:	InChI=1S/C9H20/c1-4-6-7-8-9(3)5-2/h9H,4-8H2,1-3H3
InchiKey:	SEEOMASXHIJCDV-UHFFFAOYSA-N
Formula:	C9H20
SMILES:	CCCCCC(C)CC
Mol. weight [g/mol]:	128.26
CAS:	2216-33-3

Physical Properties

Property code	Value	Unit	Source
af	0.4130		KDB
ap	348.150	K	KDB
gf	22.46	kJ/mol	Joback Method
hcg	6121.40	kJ/mol	KDB
hcn	5681.286	kJ/mol	KDB
hf	-234.37	kJ/mol	Joback Method
hfus	15.54	kJ/mol	Joback Method
hvap	44.90	kJ/mol	NIST Webbook
log10ws	-3.35		Crippen Method
logp	3.613		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2340.00	kPa	KDB
rinpol	870.00		NIST Webbook
rinpol	869.90		NIST Webbook
rinpol	870.50		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	872.30		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	871.70		NIST Webbook
rinpol	871.90		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	870.80		NIST Webbook
rinpol	871.10		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	871.10		NIST Webbook
rinpol	870.00		NIST Webbook

rinpol	871.00	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	868.00	NIST Webbook
rinpol	868.00	NIST Webbook
rinpol	869.00	NIST Webbook
rinpol	869.00	NIST Webbook
rinpol	870.00	NIST Webbook
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rinpol	871.00	NIST Webbook
rinpol	870.00	NIST Webbook
rinpol	871.93	NIST Webbook
rinpol	870.00	NIST Webbook
rinpol	869.00	NIST Webbook
rinpol	870.00	NIST Webbook
rinpol	874.00	NIST Webbook
rinpol	871.00	NIST Webbook
rinpol	873.50	NIST Webbook
rinpol	871.40	NIST Webbook
rinpol	871.40	NIST Webbook
rinpol	863.40	NIST Webbook
rinpol	869.60	NIST Webbook
rinpol	870.74	NIST Webbook
rinpol	870.98	NIST Webbook
rinpol	872.00	NIST Webbook
rinpol	872.00	NIST Webbook
rinpol	872.35	NIST Webbook
rinpol	872.61	NIST Webbook
rinpol	872.89	NIST Webbook
rinpol	871.93	NIST Webbook
rinpol	869.00	NIST Webbook
rinpol	872.56	NIST Webbook
rinpol	869.00	NIST Webbook
rinpol	867.00	NIST Webbook
rinpol	871.00	NIST Webbook
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rinpol	876.00		NIST Webbook
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rinpol	871.90		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	873.50		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	872.61		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	872.10		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	871.10		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	872.10		NIST Webbook
rinpol	870.74		NIST Webbook
rinpol	872.24		NIST Webbook
rinpol	872.20		NIST Webbook
tb	416.55 ± 0.30	K	NIST Webbook
tb	416.55 ± 0.30	K	NIST Webbook
tb	416.65 ± 1.50	K	NIST Webbook
tb	417.33 ± 0.15	K	NIST Webbook
tb	417.40	K	KDB
tb	416.00 ± 3.00	K	NIST Webbook
tb	417.36 ± 0.20	K	NIST Webbook
tb	417.33 ± 0.50	K	NIST Webbook
tb	417.40 ± 0.30	K	NIST Webbook
tb	417.40 ± 0.30	K	NIST Webbook

tb	417.33 ± 0.20	K	NIST Webbook
tb	415.75 ± 0.50	K	NIST Webbook
tb	416.55 ± 0.70	K	NIST Webbook
tc	590.00	K	KDB
tf	165.15 ± 0.10	K	NIST Webbook
tf	166.00	K	KDB
vc	0.529	m3/kmol	KDB
zc	0.2523380		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.48	J/mol×K	516.01	Joback Method
cpg	351.89	J/mol×K	571.57	Joback Method
cpg	339.92	J/mol×K	543.79	Joback Method
cpg	272.60	J/mol×K	404.88	Joback Method
cpg	287.11	J/mol×K	432.66	Joback Method
cpg	301.08	J/mol×K	460.44	Joback Method
cpg	314.53	J/mol×K	488.22	Joback Method
dvisc	0.0002341	Pa×s	404.88	Joback Method
dvisc	0.0004644	Pa×s	328.65	Joback Method
dvisc	0.0003182	Pa×s	366.76	Joback Method
dvisc	0.0108182	Pa×s	176.19	Joback Method
dvisc	0.0032357	Pa×s	214.31	Joback Method
dvisc	0.0013934	Pa×s	252.42	Joback Method
dvisc	0.0007485	Pa×s	290.53	Joback Method
hfust	16.99	kJ/mol	165.60	NIST Webbook
hvapt	36.78	kJ/mol	417.40	KDB
rfi	1.40400		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45076e+01
Coeff. B	-3.67249e+03
Coeff. C	-4.60190e+01

Temperature range (K), min.	304.28
Temperature range (K), max.	445.37

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.28140e+01
Coeff. B	-8.03661e+03
Coeff. C	-9.91643e+00
Coeff. D	5.14767e-06
Temperature range (K), min.	165.55
Temperature range (K), max.	590.15

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2216333&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=65

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=65

Legend

af: Acentric Factor

ap: Aniline Point

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

hfust: Enthalpy of fusion at a given temperature

hvap: Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility