Octane, 2-methyl-

Other names: 2-Methyloctane
Isononane
Inchi: InChI=1S/C9H20/c1-4-5-6-7-8-9(2)3/h9H,4-8H2,1-3H3
InchiKey: ZUBZATZOEPUUQF-UHFFFAOYSA-N
Formula: C9H20
SMILES: CCCCCCC(C)C
Mol. weight [g/mol]: 128.26
CAS: 3221-61-2

Physical Properties

Property code	Value	Unit	Source
af	0.4230		KDB
ap	350.650	K	KDB
gf	24.83	kJ/mol	KDB
hcg	6119.27	kJ/mol	KDB
hcn	5679.153	kJ/mol	KDB
hf	-229.20	kJ/mol	KDB
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	2310.00 ± 20.68	kPa	NIST Webbook
pc	2310.00 ± 50.00	kPa	NIST Webbook
pc	2310.00	kPa	KDB
pc	2310.00 ± 20.00	kPa	NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	887.00		NIST Webbook

rinpol	869.00	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	872.00	NIST Webbook
rinpol	868.00	NIST Webbook
rinpol	871.00	NIST Webbook
rinpol	868.00	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	856.30	NIST Webbook
rinpol	864.77	NIST Webbook
rinpol	866.60	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	865.70	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	858.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	866.00	NIST Webbook
rinpol	866.00	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	864.30	NIST Webbook
rinpol	864.70	NIST Webbook
rinpol	865.70	NIST Webbook
rinpol	865.70	NIST Webbook
rinpol	863.00	NIST Webbook
rinpol	864.80	NIST Webbook
rinpol	864.10	NIST Webbook
rinpol	864.10	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	864.30	NIST Webbook
rinpol	868.00	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	863.00	NIST Webbook
rinpol	863.00	NIST Webbook
rinpol	863.00	NIST Webbook
rinpol	864.70	NIST Webbook

rinpol	865.00	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	876.00	NIST Webbook
rinpol	866.00	NIST Webbook
rinpol	858.00	NIST Webbook
rinpol	864.90	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	863.00	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	858.00	NIST Webbook
rinpol	875.40	NIST Webbook
rinpol	868.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	858.00	NIST Webbook
rinpol	866.80	NIST Webbook
rinpol	860.20	NIST Webbook
rinpol	864.80	NIST Webbook
rinpol	856.30	NIST Webbook
rinpol	862.30	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	864.17	NIST Webbook
rinpol	864.60	NIST Webbook
rinpol	864.77	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	866.36	NIST Webbook
rinpol	866.49	NIST Webbook
rinpol	866.60	NIST Webbook
rinpol	865.63	NIST Webbook
rinpol	865.75	NIST Webbook
rinpol	865.92	NIST Webbook
rinpol	863.00	NIST Webbook
rinpol	866.50	NIST Webbook
rinpol	855.00	NIST Webbook
rinpol	861.00	NIST Webbook
rinpol	884.05	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	864.00	NIST Webbook
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rinpol	871.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	858.00		NIST Webbook
ripol	864.00		NIST Webbook
ripol	865.00		NIST Webbook
ripol	882.00		NIST Webbook
ripol	858.00		NIST Webbook
ripol	864.00		NIST Webbook
tb	416.50 ± 0.30	K	NIST Webbook
tb	416.40	K	NIST Webbook
tb	415.00 ± 3.00	K	NIST Webbook
tb	416.65 ± 1.00	K	NIST Webbook
tb	416.41 ± 0.10	K	NIST Webbook
tb	415.95 ± 0.30	K	NIST Webbook
tb	415.95 ± 0.30	K	NIST Webbook
tb	415.95 ± 0.70	K	NIST Webbook
tb	416.40 ± 0.15	K	NIST Webbook
tb	415.95 ± 0.40	K	NIST Webbook
tb	416.43	K	KDB
tb	416.41 ± 0.20	K	NIST Webbook
tb	416.50 ± 0.30	K	NIST Webbook
tb	415.25 ± 0.40	K	NIST Webbook
tb	415.95 ± 0.50	K	NIST Webbook
tc	582.80	K	KDB
tc	582.80 ± 0.10	K	NIST Webbook
tc	582.87 ± 0.30	K	NIST Webbook
tc	582.87 ± 0.20	K	NIST Webbook
tf	192.75 ± 0.15	K	NIST Webbook
tf	193.05 ± 0.20	K	NIST Webbook
tf	192.66 ± 0.10	K	NIST Webbook
tf	192.78	K	KDB
vc	0.533	m3/kmol	KDB
zc	0.2543260		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	327.48	J/mol×K	516.01	Joback Method
cpg	339.92	J/mol×K	543.79	Joback Method
cpg	351.89	J/mol×K	571.57	Joback Method
dvisc	0.0032357	Pa×s	214.31	Joback Method
dvisc	0.0013934	Pa×s	252.42	Joback Method
dvisc	0.0108182	Pa×s	176.19	Joback Method
dvisc	0.0007485	Pa×s	290.53	Joback Method
dvisc	0.0004644	Pa×s	328.65	Joback Method
dvisc	0.0003182	Pa×s	366.76	Joback Method
dvisc	0.0002341	Pa×s	404.88	Joback Method
hfust	17.99	kJ/mol	192.80	NIST Webbook
hvapt	36.65	kJ/mol	416.20	KDB
hvapt	43.20	kJ/mol	361.00	NIST Webbook
rfi	1.40080		298.15	KDB
rhol	691.60	kg/m3	323.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	699.60	kg/m3	313.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	707.60	kg/m3	303.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	715.40	kg/m3	293.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

rhol	723.20	kg/m3	283.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	649.70	kg/m3	373.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	658.20	kg/m3	363.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	666.70	kg/m3	353.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	675.10	kg/m3	343.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	683.30	kg/m3	333.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	691.40	kg/m3	323.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

rhol	699.40	kg/m3	313.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	707.40	kg/m3	303.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	715.30	kg/m3	293.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	723.20	kg/m3	283.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	713.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44193e+01
Coeff. B	-3.57795e+03
Coeff. C	-5.13690e+01
Temperature range (K), min.	304.56
Temperature range (K), max.	444.21

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.56228e+01
Coeff. B	-8.16941e+03
Coeff. C	-1.03339e+01
Coeff. D	5.46510e-06
Temperature range (K), min.	192.78
Temperature range (K), max.	586.75

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels:	https://www.doi.org/10.1021/je400274f
KDB:	https://www.cheric.org/files/research/kdb/mol/mol64.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3221612&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=64
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility