Nonane, 4-methyl-

Other names:	4-Methylnonane
	4-Methylnonane, (DL)-
	n-C3H7CH(CH3)(CH2)4CH3
Inchi:	InChI=1S/C10H22/c1-4-6-7-9-10(3)8-5-2/h10H,4-9H2,1-3H3
InchiKey:	IALRSQMWHFKJJA-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CCCCCC(C)CCC
Mol. weight [g/mol]:	142.28
CAS:	17301-94-9

Physical Properties

Property code	Value	Unit	Source
af	0.4510		KDB
ap	351.450	K	KDB
gf	30.88	kJ/mol	Joback Method
hcg	6775.57	kJ/mol	KDB
hcn	6291.439	kJ/mol	KDB
hf	-255.01	kJ/mol	Joback Method
hfus	18.13	kJ/mol	Joback Method
hvap	49.50	kJ/mol	NIST Webbook
log10ws	-3.77		Crippen Method
logp	4.003		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2140.00	kPa	KDB
rinpol	960.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	960.00		NIST Webbook

rinpol	964.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	962.50	NIST Webbook
rinpol	962.40	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	959.30	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	960.80	NIST Webbook
rinpol	965.00	NIST Webbook
rinpol	964.00	NIST Webbook
rinpol	966.00	NIST Webbook
rinpol	968.00	NIST Webbook
rinpol	963.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	960.63	NIST Webbook
rinpol	960.63	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	962.40	NIST Webbook
rinpol	963.00	NIST Webbook
rinpol	955.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	967.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	963.80	NIST Webbook
rinpol	962.10	NIST Webbook
rinpol	961.60	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	963.54	NIST Webbook
rinpol	963.12	NIST Webbook
rinpol	963.33	NIST Webbook
rinpol	963.34	NIST Webbook
rinpol	962.48	NIST Webbook
rinpol	962.63	NIST Webbook
rinpol	962.67	NIST Webbook
rinpol	955.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	963.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	964.00	NIST Webbook
rinpol	961.00	NIST Webbook

rinpol	958.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	962.80		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	960.00		NIST Webbook
sl	425.50	J/mol×K	NIST Webbook
tb	438.90 ± 0.50	K	NIST Webbook
tb	438.90	K	KDB
tb	441.15 ± 2.00	K	NIST Webbook
tb	438.85 ± 0.50	K	NIST Webbook
tb	438.90 ± 0.30	K	NIST Webbook
tb	438.90 ± 0.50	K	NIST Webbook
tb	442.15 ± 2.00	K	NIST Webbook
tc	610.50	K	KDB
tf	174.00	K	KDB
tf	174.69 ± 0.20	K	NIST Webbook
tf	171.53 ± 0.15	K	NIST Webbook
tt	174.70 ± 0.20	K	NIST Webbook
vc	0.575	m3/kmol	KDB
zc	0.2424150		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.91	J/mol×K	593.73	Joback Method
cpg	330.79	J/mol×K	455.42	Joback Method
cpg	360.07	J/mol×K	510.75	Joback Method
cpg	373.88	J/mol×K	538.41	Joback Method
cpg	387.16	J/mol×K	566.07	Joback Method
cpg	315.29	J/mol×K	427.76	Joback Method
cpg	345.71	J/mol×K	483.08	Joback Method
cpl	317.36	J/mol×K	298.10	NIST Webbook
dvisc	0.0007355	Pa×s	307.61	Joback Method
dvisc	0.0108083	Pa×s	187.46	Joback Method
dvisc	0.0032190	Pa×s	227.51	Joback Method
dvisc	0.0013777	Pa×s	267.56	Joback Method
dvisc	0.0004537	Pa×s	347.66	Joback Method
dvisc	0.0003093	Pa×s	387.71	Joback Method

dvisc	0.0002265	Pa×s	427.76	Joback Method
hfust	15.19	kJ/mol	174.70	NIST Webbook
hfust	15.19	kJ/mol	174.70	NIST Webbook
hvapt	38.79	kJ/mol	438.90	KDB
rfi	1.40950		298.15	KDB
rhol	684.94	kg/m3	353.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	708.82	kg/m3	323.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	728.35	kg/m3	298.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	668.81	kg/m3	373.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	647.86	kg/m3	398.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	626.00	kg/m3	423.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	676.88	kg/m3	363.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	689.00	kg/m3	348.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane

rhol	680.92	kg/m3	358.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane	
rhol	688.94	kg/m3	348.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane	
rhol	692.92	kg/m3	343.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane	
rhol	696.87	kg/m3	338.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane	
rhol	700.81	kg/m3	333.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane	
rhol	704.73	kg/m3	328.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane	
rhol	708.63	kg/m3	323.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane	
rhol	712.53	kg/m3	318.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane	

rhol	716.40	kg/m3	313.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	720.25	kg/m3	308.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	724.10	kg/m3	303.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	731.74	kg/m3	293.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	735.55	kg/m3	288.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	739.36	kg/m3	283.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
rhol	727.93	kg/m3	298.15	Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane
sfust	86.94	J/mol×K	174.70	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47150e+01
Coeff. B	-3.97462e+03
Coeff. C	-4.51930e+01
Temperature range (K), min.	320.68
Temperature range (K), max.	467.87

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.38814e+01
Coeff. B	-8.08283e+03
Coeff. C	-8.47077e+00
Coeff. D	3.60829e-06
Temperature range (K), min.	174.45
Temperature range (K), max.	610.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid Viscosity and Interfacial Tension of Binary and Ternary Mixtures Containing n-Octacosane by Surface Light Scattering:	https://www.doi.org/10.1021/acs.jced.8b01139
Viscosity and Surface Tension of Branched Alkanes 2-Methylnonane and 4-Methylnonane:	https://www.doi.org/10.1021/acs.jced.8b00163
Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=100
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17301949&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=100
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
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
ap:	Aniline Point
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility