Nonane, 3-methyl-

Other names:	3-Methylnonane
	3-Methylnonane, (DL)-
Inchi:	InChI=1S/C10H22/c1-4-6-7-8-9-10(3)5-2/h10H,4-9H2,1-3H3
InchiKey:	PLZDDPSCZHRBOY-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CCCCCCC(C)CC
Mol. weight [g/mol]:	142.28
CAS:	5911-04-6

Physical Properties

Property code	Value	Unit	Source
af	0.4510		KDB
ap	351.350	K	KDB
gf	30.88	kJ/mol	Joback Method
hcg	6775.15	kJ/mol	KDB
hcn	6291.021	kJ/mol	KDB
hf	-255.01	kJ/mol	Joback Method
hfus	18.13	kJ/mol	Joback Method
hvap	50.20	kJ/mol	NIST Webbook
hvap	49.72	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	976.00		NIST Webbook
rinpol	971.20		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	970.40		NIST Webbook
rinpol	970.40		NIST Webbook
rinpol	970.60		NIST Webbook
rinpol	972.50		NIST Webbook
rinpol	970.40		NIST Webbook
rinpol	971.30		NIST Webbook
rinpol	969.60		NIST Webbook
rinpol	970.20		NIST Webbook
rinpol	973.00		NIST Webbook

rinpol	958.00	NIST Webbook
rinpol	970.42	NIST Webbook
rinpol	970.42	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	977.00	NIST Webbook
rinpol	971.92	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	971.00	NIST Webbook
rinpol	977.20	NIST Webbook
rinpol	979.00	NIST Webbook
rinpol	969.00	NIST Webbook
rinpol	972.00	NIST Webbook
rinpol	976.00	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	972.80	NIST Webbook
rinpol	969.00	NIST Webbook
rinpol	971.20	NIST Webbook
rinpol	970.50	NIST Webbook
rinpol	971.70	NIST Webbook
rinpol	974.20	NIST Webbook
rinpol	972.00	NIST Webbook
rinpol	971.00	NIST Webbook
rinpol	971.80	NIST Webbook
rinpol	972.15	NIST Webbook
rinpol	972.23	NIST Webbook
rinpol	971.40	NIST Webbook
rinpol	971.74	NIST Webbook
rinpol	971.85	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	968.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	971.00	NIST Webbook
rinpol	969.00	NIST Webbook
rinpol	972.00	NIST Webbook
rinpol	975.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	974.00	NIST Webbook
rinpol	973.00	NIST Webbook
rinpol	972.10	NIST Webbook
rinpol	967.00	NIST Webbook
rinpol	970.00	NIST Webbook

rinpol	964.00	NIST Webbook
rinpol	976.00	NIST Webbook
rinpol	966.00	NIST Webbook
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rinpol	970.40	NIST Webbook
rinpol	971.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	971.30	NIST Webbook
ripol	983.00	NIST Webbook
ripol	969.00	NIST Webbook
ripol	983.00	NIST Webbook
ripol	965.00	NIST Webbook
ripol	969.00	NIST Webbook

sl	427.20	J/mol×K	NIST Webbook
tb	441.00	K	KDB
tc	613.40	K	KDB
tc	613.60	K	NIST Webbook
tf	188.00	K	KDB
tf	188.49 ± 0.20	K	NIST Webbook
tf	183.15 ± 0.50	K	NIST Webbook
tf	188.29 ± 0.20	K	NIST Webbook
tt	188.50 ± 0.20	K	NIST Webbook
vc	0.582	m3/kmol	KDB
zc	0.2442060		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.91	J/mol×K	593.73	Joback Method
cpg	387.16	J/mol×K	566.07	Joback Method
cpg	315.29	J/mol×K	427.76	Joback Method
cpg	330.79	J/mol×K	455.42	Joback Method
cpg	345.71	J/mol×K	483.08	Joback Method
cpg	360.07	J/mol×K	510.75	Joback Method
cpg	373.88	J/mol×K	538.41	Joback Method
cpl	308.99	J/mol×K	298.10	NIST Webbook
dvisc	0.0002265	Pa×s	427.76	Joback Method
dvisc	0.0003093	Pa×s	387.71	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	0.0007355	Pa×s	307.61	Joback Method
dvisc	0.0004537	Pa×s	347.66	Joback Method
hfust	18.70	kJ/mol	188.50	NIST Webbook
hfust	18.70	kJ/mol	188.50	NIST Webbook
hvapt	45.10 ± 0.20	kJ/mol	358.00	NIST Webbook
hvapt	46.20 ± 0.20	kJ/mol	343.00	NIST Webbook
hvapt	39.12	kJ/mol	441.00	KDB
hvapt	38.26	kJ/mol	441.00	NIST Webbook
hvapt	47.30 ± 0.20	kJ/mol	328.00	NIST Webbook
rfi	1.41030		298.15	KDB
sfust	99.20	J/mol×K	188.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45072e+01
Coeff. B	-3.79773e+03
Coeff. C	-5.69090e+01
Temperature range (K), min.	323.99
Temperature range (K), max.	469.90

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.11505e+02
Coeff. B	-9.76977e+03
Coeff. C	-1.41847e+01
Coeff. D	8.42650e-06
Temperature range (K), min.	188.35
Temperature range (K), max.	613.00

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=99

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5911046&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=99

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

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

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
rinpol:	Non-polar retention indices
ripol:	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