Nonane, 5-methyl-

Other names: 5-Methylnonane
Inchi: InChI=1S/C10H22/c1-4-6-8-10(3)9-7-5-2/h10H,4-9H2,1-3H3
InchiKey: TYSIILFJZXHVPU-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCCCC(C)CCCC
Mol. weight [g/mol]: 142.28
CAS: 15869-85-9

Physical Properties

Property code	Value	Unit	Source
af	0.4520		KDB
ap	351.050	K	KDB
chl	-6771.40 ± 1.60	kJ/mol	NIST Webbook
gf	30.88	kJ/mol	Joback Method
hcg	6775.74	kJ/mol	KDB
hcn	6291.606	kJ/mol	KDB
hf	-258.60	kJ/mol	NIST Webbook
hfl	-307.90 ± 1.60	kJ/mol	NIST Webbook
hfus	18.13	kJ/mol	Joback Method
hvap	49.35	kJ/mol	NIST Webbook
hvap	49.80	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	958.60		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	962.10		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	961.48		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	960.97		NIST Webbook
rinpol	957.00		NIST Webbook

rinpol	961.10	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	957.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	966.00	NIST Webbook
rinpol	965.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	964.00	NIST Webbook
rinpol	964.00	NIST Webbook
rinpol	960.80	NIST Webbook
rinpol	960.80	NIST Webbook
rinpol	956.00	NIST Webbook
rinpol	957.40	NIST Webbook
rinpol	960.80	NIST Webbook
rinpol	954.00	NIST Webbook
rinpol	957.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	957.00	NIST Webbook
rinpol	967.80	NIST Webbook
rinpol	957.00	NIST Webbook
rinpol	962.10	NIST Webbook
rinpol	958.10	NIST Webbook
rinpol	959.80	NIST Webbook
rinpol	963.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	961.48	NIST Webbook
rinpol	961.76	NIST Webbook
rinpol	961.62	NIST Webbook
rinpol	960.91	NIST Webbook
rinpol	961.01	NIST Webbook
rinpol	960.97	NIST Webbook
rinpol	966.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	959.00	NIST Webbook
rinpol	960.00	NIST Webbook
ripol	960.00	NIST Webbook
ripol	960.00	NIST Webbook

sl	423.80	J/mol×K	NIST Webbook
tb	438.30	K	KDB
tb	438.30	K	NIST Webbook
tb	438.30	K	NIST Webbook
tb	438.30 ± 0.30	K	NIST Webbook
tb	435.65 ± 2.00	K	NIST Webbook
tb	438.15 ± 2.00	K	NIST Webbook
tc	609.60	K	KDB
tc	609.80	K	NIST Webbook
tf	185.00	K	KDB
tf	186.70 ± 0.20	K	NIST Webbook
tf	186.35 ± 0.15	K	NIST Webbook
tt	186.70 ± 0.01	K	NIST Webbook
vc	0.573	m3/kmol	KDB
zc	0.2419280		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.91	J/mol×K	593.73	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
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
cpl	314.43	J/mol×K	298.10	NIST Webbook
dvisc	0.0004537	Pa×s	347.66	Joback Method
dvisc	0.0007355	Pa×s	307.61	Joback Method
dvisc	0.0013777	Pa×s	267.56	Joback Method
dvisc	0.0032190	Pa×s	227.51	Joback Method
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
hfust	16.64	kJ/mol	186.70	NIST Webbook
hfust	16.65	kJ/mol	186.70	NIST Webbook
hfust	16.65	kJ/mol	186.70	NIST Webbook
hvapt	45.90 ± 0.20	kJ/mol	343.00	NIST Webbook
hvapt	38.14	kJ/mol	438.30	NIST Webbook
hvapt	38.70	kJ/mol	438.30	KDB
hvapt	44.60 ± 0.20	kJ/mol	358.00	NIST Webbook

hvapt	47.00 ± 0.20	kJ/mol	328.00	NIST Webbook
rfi	1.41000		298.15	KDB
sfust	89.13	J/mol×K	186.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44953e+01
Coeff. B	-3.77885e+03
Coeff. C	-5.57070e+01
Temperature range (K), min.	321.68
Temperature range (K), max.	467.18

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.03449e+02
Coeff. B	-9.43079e+03
Coeff. C	-1.29252e+01
Coeff. D	6.82316e-06
Temperature range (K), min.	185.45
Temperature range (K), max.	610.00

Sources

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol101.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15869859&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=101

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
chl:	Standard liquid enthalpy of combustion
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
hfl:	Liquid phase 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