

2-Nonanol

Other names:	1-Methyl-1-octanol NONAN-2-OL Nonanol-(2) n-Nonan-2-ol
Inchi:	InChI=1S/C9H20O/c1-3-4-5-6-7-8-9(2)10/h9-10H,3-8H2,1-2H3
InchiKey:	NGDNVOAEIVQRFH-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCCCCCC(C)O
Mol. weight [g/mol]:	144.25
CAS:	628-99-9

Physical Properties

Property code	Value	Unit	Source
cpl	356.31	J/mol×K	Vapour pressures and heat capacity measurements on the C7 C9 secondary aliphatic alcohols
gf	-114.36	kJ/mol	Joback Method
hf	-386.60	kJ/mol	Joback Method
hfus	19.63	kJ/mol	Joback Method
hvap	72.90 ± 0.60	kJ/mol	NIST Webbook
log10ws	-2.74		Estimated Solubility Method
log10ws	-2.74		Aqueous Solubility Prediction Method
logp	2.728		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2530.00 ± 20.00	kPa	NIST Webbook
pc	2530.00 ± 20.00	kPa	NIST Webbook
pc	2530.00 ± 50.00	kPa	NIST Webbook
pc	2530.00	kPa	KDB
rhoc	251.00 ± 7.21	kg/m3	NIST Webbook
rhoc	251.00 ± 5.77	kg/m3	NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1085.00		NIST Webbook

rinpol	1102.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1101.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1076.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1072.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1108.70	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1089.00	NIST Webbook
ripol	1528.00	NIST Webbook
ripol	1521.00	NIST Webbook
ripol	1484.00	NIST Webbook

ripol	1521.00	NIST Webbook
ripol	1518.00	NIST Webbook
ripol	1499.00	NIST Webbook
ripol	1521.00	NIST Webbook
ripol	1509.00	NIST Webbook
ripol	1488.00	NIST Webbook
ripol	1508.00	NIST Webbook
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ripol	1508.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1499.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1518.00		NIST Webbook
ripol	1538.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1528.00		NIST Webbook
tb	465.65 ± 5.00	K	NIST Webbook
tb	466.70	K	NIST Webbook
tb	473.15 ± 5.00	K	NIST Webbook
tb	471.50 ± 0.60	K	NIST Webbook
tb	471.35 ± 1.00	K	NIST Webbook
tb	466.15 ± 3.00	K	NIST Webbook
tb	466.65 ± 3.00	K	NIST Webbook
tb	466.65 ± 5.00	K	NIST Webbook
tb	466.65 ± 3.00	K	NIST Webbook
tb	470.65 ± 3.00	K	NIST Webbook
tb	468.65 ± 3.00	K	NIST Webbook
tc	649.10 ± 0.30	K	NIST Webbook
tc	649.60	K	KDB
tc	650.00 ± 1.00	K	NIST Webbook
tc	650.10 ± 0.60	K	NIST Webbook
tc	650.10 ± 0.60	K	NIST Webbook
tc	649.50	K	NIST Webbook
tf	237.98	K	Aqueous Solubility Prediction Method
vc	0.575	m3/kmol	NIST Webbook
vc	0.575	m3/kmol	KDB
zc	0.2693430		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.58	J/mol×K	497.06	Joback Method
cpg	347.30	J/mol×K	524.07	Joback Method
cpg	359.54	J/mol×K	551.09	Joback Method

cpg	371.30	J/mol×K	578.10	Joback Method
cpg	382.60	J/mol×K	605.11	Joback Method
cpg	393.45	J/mol×K	632.13	Joback Method
cpg	403.87	J/mol×K	659.14	Joback Method
dvisc	0.0131188	Pa×s	280.35	Joback Method
dvisc	0.0878509	Pa×s	237.01	Joback Method
dvisc	0.0032599	Pa×s	323.69	Joback Method
dvisc	0.0011254	Pa×s	367.03	Joback Method
dvisc	0.0004864	Pa×s	410.38	Joback Method
dvisc	0.0002468	Pa×s	453.72	Joback Method
dvisc	0.0001409	Pa×s	497.06	Joback Method
hvapt	79.60	kJ/mol	303.00	NIST Webbook
hvapt	55.50	kJ/mol	417.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64188e+01
Coeff. B	-4.61124e+03
Coeff. C	-7.82320e+01
Temperature range (K), min.	364.09
Temperature range (K), max.	493.39

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.35307e+02
Coeff. B	-1.31543e+04
Coeff. C	-1.69302e+01
Coeff. D	6.49313e-06
Temperature range (K), min.	238.51
Temperature range (K), max.	623.00

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=847
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=847
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628999&Units=SI
Vapour pressures and heat capacity measurements on the C7 C9 secondary aliphatic alcohols:	https://www.doi.org/10.1016/j.jct.2006.10.007

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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