3-Nonanol

Other names: Hexylethylcarbinol
nonan-3-ol
Inchi: InChI=1S/C9H20O/c1-3-5-6-7-8-9(10)4-2/h9-10H,3-8H2,1-2H3
InchiKey: GYSCXPVAKHVAAY-UHFFFAOYSA-N
Formula: C9H20O
SMILES: CCCCCCC(O)CC
Mol. weight [g/mol]: 144.25
CAS: 624-51-1

Physical Properties

Property code	Value	Unit	Source
cpl	373.62	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	70.90 ± 0.30	kJ/mol	NIST Webbook
log10ws	-2.97		Crippen Method
logp	2.728		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rhoc	249.56 ± 5.77	kg/m3	NIST Webbook
rhoc	249.56	kg/m3	NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1069.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1461.00		NIST Webbook
ripol	1459.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1496.00		NIST Webbook
tb	467.90 ± 3.00	K	NIST Webbook

tc	648.00 ± 1.00	K	NIST Webbook
tc	648.00	K	NIST Webbook
tc	648.00 ± 0.30	K	NIST Webbook
tf	237.01	K	Joback Method
vc	0.577	m3/kmol	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.45	J/mol×K	632.13	Joback Method
cpg	403.87	J/mol×K	659.14	Joback Method
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
dvisc	0.0001409	Pa×s	497.06	Joback Method
dvisc	0.0002468	Pa×s	453.72	Joback Method
dvisc	0.0878509	Pa×s	237.01	Joback Method
dvisc	0.0131188	Pa×s	280.35	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
hvapt	57.10	kJ/mol	417.00	NIST Webbook
hvapt	75.50	kJ/mol	313.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.69298e+01
Coeff. B	-5.26910e+03
Coeff. C	-3.99180e+01
Temperature range (K), min.	356.53
Temperature range (K), max.	493.43

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and heat capacity measurements on the C7 C9 secondary aliphatic alcohols:	https://www.doi.org/10.1016/j.jct.2006.10.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C624511&Units=SI

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