1-Hexanol, 3,5,5-trimethyl-

Other names:	3,5,5-Trimethyl n-hexanol
	3,5,5-Trimethyl-1-hexanol
	3,5,5-Trimethylhexan-1-ol
	3,5,5-Trimethylhexanol
	3,5,5-Trimethylhexyl alcohol
	NSC 83151
	NSC 97226
	Nonylol
	i-Nonyl alcohol
Inchi:	InChI=1S/C9H20O/c1-8(5-6-10)7-9(2,3)4/h8,10H,5-7H2,1-4H3
InchiKey:	BODRLKRKPXBDBN-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CC(CCO)CC(C)(C)C
Mol. weight [g/mol]:	144.25
CAS:	3452-97-9

Physical Properties

Property code	Value	Unit	Source
chl	-5943.00 ± 3.00	kJ/mol	NIST Webbook
gf	-111.52	kJ/mol	Joback Method
hf	-395.35	kJ/mol	Joback Method
hfl	-456.90	kJ/mol	NIST Webbook
hfus	12.22	kJ/mol	Joback Method
hvap	67.90 ± 0.40	kJ/mol	NIST Webbook
log10ws	-2.37		Crippen Method
logp	2.441		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1041.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1049.00		NIST Webbook
ripol	1480.00		NIST Webbook
tb	464.15 ± 4.00	K	NIST Webbook
tb	466.05 ± 3.00	K	NIST Webbook
tb	466.65 ± 4.00	K	NIST Webbook
tb	463.15 ± 4.00	K	NIST Webbook
tb	467.20	K	NIST Webbook

tc	664.90	K	Joback Method
tf	239.43	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.41	J/mol×K	664.90	Joback Method
cpg	351.13	J/mol×K	522.34	Joback Method
cpg	364.17	J/mol×K	550.85	Joback Method
cpg	376.59	J/mol×K	579.36	Joback Method
cpg	388.42	J/mol×K	607.88	Joback Method
cpg	399.69	J/mol×K	636.39	Joback Method
cpg	337.46	J/mol×K	493.83	Joback Method
dvisc	0.1242076	Pa×s	239.43	Joback Method
dvisc	0.0170986	Pa×s	281.83	Joback Method
dvisc	0.0039538	Pa×s	324.23	Joback Method
dvisc	0.0012828	Pa×s	366.63	Joback Method
dvisc	0.0005256	Pa×s	409.03	Joback Method
dvisc	0.0002546	Pa×s	451.43	Joback Method
dvisc	0.0001397	Pa×s	493.83	Joback Method
pvap	6.72e-03	kPa	288.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	9.15e-03	kPa	291.30	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols

pvap	0.01	kPa	294.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.02	kPa	297.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.02	kPa	300.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.03	kPa	303.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols

pvap	0.04	kPa	306.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.05	kPa	309.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.06	kPa	312.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.08	kPa	315.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	

pvap	0.10	kPa	318.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.13	kPa	321.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.16	kPa	324.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62921e+01
Coeff. B	-4.62819e+03
Coeff. C	-7.07400e+01
Temperature range (K), min.	359.92
Temperature range (K), max.	492.23

Sources

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=C3452979&Units=SI
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
Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols:	https://www.doi.org/10.1021/je049561m

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
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