2-Hexanol, 2-methyl-

Other names:	1,1-Dimethyl-1-pentanol
	2-Methyl-2-hexanol
	2-Methyl-2-hexanol
	2-Methyl-2-hydroxyhexane
	2-methylhexan-2-ol
	Butyldimethylcarbinol
	Methyl-2 hexanol-2
Inchi:	InChI=1S/C7H16O/c1-4-5-6-7(2,3)8/h8H,4-6H2,1-3H3
InchiKey:	KRIMXCDMVRMCTC-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCCC(C)(C)O
Mol. weight [g/mol]:	116.20
CAS:	625-23-0

Physical Properties

Property code	Value	Unit	Source
gf	-125.92	kJ/mol	Joback Method
hf	-348.79	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	58.60 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.08		Estimated Solubility Method
log10ws	-1.08		Aqueous Solubility Prediction Method
logp	1.948		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
rinpol	822.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	785.70		NIST Webbook
rinpol	786.10		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	782.40		NIST Webbook

rinpol	822.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	817.00		NIST Webbook
ripol	1180.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1188.00		NIST Webbook
ripol	1196.00		NIST Webbook
tb	414.65 ± 2.00	K	NIST Webbook
tb	414.70	K	NIST Webbook
tb	415.90 ± 1.00	K	NIST Webbook
tb	412.15 ± 3.00	K	NIST Webbook
tb	416.25 ± 0.50	K	NIST Webbook
tb	415.10 ± 1.00	K	NIST Webbook
tb	410.65 ± 2.00	K	NIST Webbook
tb	416.25 ± 0.50	K	NIST Webbook
tb	415.15 ± 1.00	K	NIST Webbook
tb	414.15 ± 2.00	K	NIST Webbook
tc	618.48	K	Joback Method
tf	231.89	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.34	J/mol×K	618.48	Joback Method
cpg	262.01	J/mol×K	476.84	Joback Method
cpg	273.08	J/mol×K	505.17	Joback Method
cpg	283.62	J/mol×K	533.50	Joback Method
cpg	293.67	J/mol×K	561.82	Joback Method
cpg	303.23	J/mol×K	590.15	Joback Method
cpg	250.39	J/mol×K	448.51	Joback Method
cpl	279.80	J/mol×K	275.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	286.60	J/mol×K	280.00	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	286.60	J/mol×K	280.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	293.90	J/mol×K	285.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	293.80	J/mol×K	285.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	301.40	J/mol×K	290.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	301.40	J/mol×K	290.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	309.00	J/mol×K	295.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	308.90	J/mol×K	295.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	316.30	J/mol×K	300.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	316.20	J/mol×K	300.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	323.60	J/mol×K	305.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	323.50	J/mol×K	305.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	330.60	J/mol×K	310.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	330.50	J/mol×K	310.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	337.30	J/mol×K	315.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	337.20	J/mol×K	315.00	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	343.60	J/mol×K	320.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	343.60	J/mol×K	320.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	349.40	J/mol×K	325.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	349.40	J/mol×K	325.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	354.60	J/mol×K	330.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	354.50	J/mol×K	330.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	359.10	J/mol×K	335.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	359.00	J/mol×K	335.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	363.20	J/mol×K	340.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	363.00	J/mol×K	340.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	367.20	J/mol×K	345.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	366.80	J/mol×K	345.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	370.70	J/mol×K	349.99	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	370.20	J/mol×K	350.00	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	373.20	J/mol×K	355.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	372.90	J/mol×K	355.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	375.20	J/mol×K	360.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	374.90	J/mol×K	360.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	376.70	J/mol×K	365.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	376.40	J/mol×K	365.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	377.40	J/mol×K	370.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	377.20	J/mol×K	370.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	378.00	J/mol×K	375.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	377.60	J/mol×K	375.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	378.10	J/mol×K	379.98	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	279.80	J/mol×K	275.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	377.70	J/mol×K	382.70	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	273.30	J/mol×K	270.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	273.30	J/mol×K	270.00	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	267.20	J/mol×K	265.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	267.20	J/mol×K	265.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	263.70	J/mol×K	261.95	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	377.80	J/mol×K	380.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	263.30	J/mol×K	261.57	Calorimetric and FTIR study of selected aliphatic heptanols
dvisc	0.0002207	Pa×s	448.51	Joback Method
dvisc	0.0985996	Pa×s	231.89	Joback Method
dvisc	0.0179763	Pa×s	267.99	Joback Method
dvisc	0.0049095	Pa×s	304.10	Joback Method
dvisc	0.0017661	Pa×s	340.20	Joback Method
dvisc	0.0007730	Pa×s	376.30	Joback Method
dvisc	0.0003910	Pa×s	412.41	Joback Method
hvapt	54.50	kJ/mol	363.00	NIST Webbook
pvap	0.16	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	0.21	kPa	294.30	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	0.21	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	0.12	kPa	288.30	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	0.37	kPa	301.30	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	0.45	kPa	304.30	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	0.52	kPa	306.20	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	0.10	kPa	285.30	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	0.07	kPa	282.40	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	279.50	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	276.50	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	274.80	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	274.40	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	0.29	kPa	298.30	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	327.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56175e+01
Coeff. B	-3.67654e+03
Coeff. C	-7.97450e+01
Temperature range (K), min.	319.57
Temperature range (K), max.	436.48

Sources

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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C625230&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Calorimetric and FTIR study of selected aliphatic heptanols:	https://www.doi.org/10.1016/j.fluid.2016.04.003

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume