3-Hexanol, 2-methyl-

Other names:	1-Isopropyl-1-butanol
	2-Methyl-3-hexanol
	2-Methylhexan-3-ol
	5-Methyl-4-hexanol
Inchi:	InChI=1S/C7H16O/c1-4-5-7(8)6(2)3/h6-8H,4-5H2,1-3H3
InchiKey:	RGRUUTLDBCWYBL-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCC(O)C(C)C
Mol. weight [g/mol]:	116.20
CAS:	617-29-8

Physical Properties

Property code	Value	Unit	Source
gf	-133.64	kJ/mol	Joback Method
hf	-350.60	kJ/mol	Joback Method
hfus	10.93	kJ/mol	Joback Method
hvap	47.08	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.803		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	858.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	858.00		NIST Webbook
tb	414.65 ± 3.00	K	NIST Webbook
tb	414.65 ± 3.00	K	NIST Webbook
tb	427.15 ± 5.00	K	NIST Webbook
tb	417.00 ± 3.00	K	NIST Webbook
tb	413.90 ± 2.00	K	NIST Webbook
tb	418.65 ± 3.00	K	NIST Webbook
tc	618.05	K	Joback Method

tf	199.47	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.03	J/mol×K	450.86	Joback Method
cpg	259.20	J/mol×K	478.73	Joback Method
cpg	269.95	J/mol×K	506.59	Joback Method
cpg	280.27	J/mol×K	534.46	Joback Method
cpg	290.18	J/mol×K	562.32	Joback Method
cpg	299.70	J/mol×K	590.19	Joback Method
cpg	308.82	J/mol×K	618.05	Joback Method
cpl	270.50	J/mol×K	261.93	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	270.20	J/mol×K	262.30	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	273.80	J/mol×K	265.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	274.50	J/mol×K	265.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	280.80	J/mol×K	270.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	281.30	J/mol×K	270.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	288.30	J/mol×K	275.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	288.80	J/mol×K	275.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	295.90	J/mol×K	280.00	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	296.40	J/mol×K	280.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	303.70	J/mol×K	285.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	304.20	J/mol×K	285.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	311.90	J/mol×K	290.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	312.50	J/mol×K	290.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	319.90	J/mol×K	295.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	320.60	J/mol×K	295.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	327.40	J/mol×K	300.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	328.40	J/mol×K	300.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	334.80	J/mol×K	305.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	335.60	J/mol×K	305.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	341.80	J/mol×K	310.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	342.60	J/mol×K	310.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	348.60	J/mol×K	315.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	349.10	J/mol×K	315.00	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	353.90	J/mol×K	320.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	354.60	J/mol×K	320.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	372.30	J/mol×K	380.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	359.50	J/mol×K	325.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	362.80	J/mol×K	330.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	363.70	J/mol×K	330.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	366.10	J/mol×K	335.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	367.20	J/mol×K	335.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	368.40	J/mol×K	340.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	369.60	J/mol×K	340.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	370.50	J/mol×K	345.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	371.70	J/mol×K	345.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	372.50	J/mol×K	350.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	373.70	J/mol×K	350.00	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	373.90	J/mol×K	355.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	375.10	J/mol×K	355.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	374.50	J/mol×K	360.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	375.70	J/mol×K	360.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	374.60	J/mol×K	365.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	370.80	J/mol×K	382.85	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	374.20	J/mol×K	370.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	375.30	J/mol×K	370.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	373.10	J/mol×K	375.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	374.20	J/mol×K	375.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	371.60	J/mol×K	380.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	358.70	J/mol×K	325.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	370.50	J/mol×K	382.83	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	375.80	J/mol×K	365.00	Calorimetric and FTIR study of selected aliphatic heptanols
dvisc	0.4386858	Pa×s	199.47	Joback Method
dvisc	0.0395574	Pa×s	241.37	Joback Method
dvisc	0.0072680	Pa×s	283.27	Joback Method

dvisc	0.0020664	Pa×s	325.16	Joback Method
dvisc	0.0007829	Pa×s	367.06	Joback Method
dvisc	0.0003619	Pa×s	408.96	Joback Method
dvisc	0.0001931	Pa×s	450.86	Joback Method
hvapt	55.70	kJ/mol	371.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.20	K	102.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54383e+01
Coeff. B	-3.59470e+03
Coeff. C	-8.57700e+01
Temperature range (K), min.	323.03
Temperature range (K), max.	440.74

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=C617298&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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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