2-Hexanol, 5-methyl-

Other names:	2-Methyl-5-hexanol
	5-Methyl-2-hexanol
	5-Methylhexanol-(2)
	5-methylhexan-2-ol
Inchi:	InChI=1S/C7H16O/c1-6(2)4-5-7(3)8/h6-8H,4-5H2,1-3H3
InchiKey:	ZDVJGWXFXGJSIU-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CC(C)CCC(C)O
Mol. weight [g/mol]:	116.20
CAS:	627-59-8

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	-1.38		Aqueous Solubility Prediction Method
logp	1.803		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	422.00 ± 5.00	K	NIST Webbook
tb	422.15 ± 3.00	K	NIST Webbook
tb	422.15 ± 3.00	K	NIST Webbook
tb	422.20	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	255.40	J/mol×K	262.05	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	254.70	J/mol×K	261.83	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	257.70	J/mol×K	265.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	258.60	J/mol×K	265.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	263.10	J/mol×K	270.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	263.90	J/mol×K	270.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	268.60	J/mol×K	275.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	269.50	J/mol×K	275.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	274.40	J/mol×K	280.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	275.20	J/mol×K	280.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	280.30	J/mol×K	285.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	281.10	J/mol×K	285.00	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	286.30	J/mol×K	290.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	287.10	J/mol×K	290.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	292.10	J/mol×K	295.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	292.90	J/mol×K	295.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	297.70	J/mol×K	300.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	298.60	J/mol×K	300.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	303.40	J/mol×K	305.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	304.10	J/mol×K	305.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	308.90	J/mol×K	310.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	309.60	J/mol×K	310.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	314.20	J/mol×K	315.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	315.00	J/mol×K	315.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	319.40	J/mol×K	320.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	320.40	J/mol×K	320.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	368.80	J/mol×K	379.90	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	325.60	J/mol×K	325.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	329.80	J/mol×K	330.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	330.70	J/mol×K	330.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	334.50	J/mol×K	335.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	335.50	J/mol×K	335.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	339.10	J/mol×K	340.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	340.10	J/mol×K	340.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	343.80	J/mol×K	345.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	344.80	J/mol×K	345.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	348.50	J/mol×K	350.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	349.60	J/mol×K	350.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	352.90	J/mol×K	355.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	354.00	J/mol×K	355.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	356.80	J/mol×K	360.00	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	358.00	J/mol×K	360.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	371.70	J/mol×K	382.84	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	361.50	J/mol×K	365.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	363.30	J/mol×K	370.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	364.70	J/mol×K	370.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	366.30	J/mol×K	375.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	367.70	J/mol×K	375.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	324.70	J/mol×K	325.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	370.30	J/mol×K	380.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	360.20	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	49.40	kJ/mol	388.00	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62024e+01
Coeff. B	-4.17747e+03
Coeff. C	-6.15770e+01
Temperature range (K), min.	324.07
Temperature range (K), max.	445.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627598&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
Calorimetric and FTIR study of selected aliphatic heptanols:	https://www.doi.org/10.1016/j.fluid.2016.04.003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume