

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/molxK	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	Paxs	199.47	Joback Method
dvisc	0.0395574	Paxs	241.37	Joback Method
dvisc	0.0072680	Paxs	283.27	Joback Method
dvisc	0.0020664	Paxs	325.16	Joback Method
dvisc	0.0007829	Paxs	367.06	Joback Method
dvisc	0.0003619	Paxs	408.96	Joback Method
dvisc	0.0001931	Paxs	450.86	Joback Method
hvapt	49.40	kJ/mol	388.00	NIST Webbook

Correlations

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

Calorimetric and FTIR study of selected <https://www.doi.org/10.1016/j.fluid.2016.04.003>

aliphatic heptanols:

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

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>

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

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