3-Heptanol

Other names:	1-Ethyl-1-pentanol
	3-Hydroxyheptane
	CH3(CH2)3CHOHCH2CH3
	DL-3-Heptanol
	Ethyl-n-butylcarbinol
	Ethylbutylcarbinol
	Heptan-3-ol
	Heptanol-3
	NSC 2586
	n-Heptan-3-ol
Inchi:	InChI=1S/C7H16O/c1-3-5-6-7(8)4-2/h7-8H,3-6H2,1-2H3
InchiKey:	RZKSECIXORKHQS-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCCC(O)CC
Mol. weight [g/mol]:	116.20
CAS:	589-82-2

Physical Properties

Property code	Value	Unit	Source
gf	-131.20	kJ/mol	Joback Method
hf	-355.30 ± 2.10	kJ/mol	NIST Webbook
hfl	-416.80 ± 0.67	kJ/mol	NIST Webbook
hfus	14.45	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
ie	9.68 ± 0.03	eV	NIST Webbook
ie	10.01	eV	NIST Webbook
log10ws	-1.47		Aqueous Solubility Prediction Method
log10ws	-1.47		Estimated Solubility Method
logp	1.948		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rhoc	268.43	kg/m3	NIST Webbook
rhoc	268.43 ± 19.75	kg/m3	NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	882.00		NIST Webbook

rinpol	892.10		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	883.80		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	892.10		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	877.90		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	885.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1292.00		NIST Webbook
ripol	1290.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1290.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1306.00		NIST Webbook
tb	425.15 ± 3.00	K	NIST Webbook
tb	426.65 ± 3.00	K	NIST Webbook
tb	429.55 ± 0.50	K	NIST Webbook
tb	425.15 ± 3.00	K	NIST Webbook
tb	426.15 ± 2.00	K	NIST Webbook
tc	605.40 ± 0.25	K	NIST Webbook
tc	605.40 ± 0.50	K	NIST Webbook
tc	605.30	K	NIST Webbook
tf	214.47	K	Joback Method
vc	0.434	m3/kmol	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	247.92	J/mol×K	451.30	Joback Method
cpg	258.79	J/mol×K	478.59	Joback Method
cpg	269.25	J/mol×K	505.89	Joback Method
cpg	279.32	J/mol×K	533.18	Joback Method
cpg	289.00	J/mol×K	560.47	Joback Method
cpg	298.30	J/mol×K	587.77	Joback Method
cpg	307.23	J/mol×K	615.06	Joback Method
cpl	274.70	J/mol×K	261.36	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	274.70	J/mol×K	261.41	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	278.90	J/mol×K	265.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	278.60	J/mol×K	265.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	284.30	J/mol×K	270.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	284.00	J/mol×K	270.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	289.80	J/mol×K	275.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	289.30	J/mol×K	275.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	295.40	J/mol×K	280.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	294.70	J/mol×K	280.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	300.80	J/mol×K	285.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	300.10	J/mol×K	285.00	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	306.50	J/mol×K	290.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	305.60	J/mol×K	290.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	312.10	J/mol×K	295.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	311.00	J/mol×K	295.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	317.40	J/mol×K	300.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	316.40	J/mol×K	300.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	323.00	J/mol×K	305.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	322.10	J/mol×K	305.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	328.80	J/mol×K	310.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	327.80	J/mol×K	310.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	334.30	J/mol×K	315.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	332.70	J/mol×K	315.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	339.90	J/mol×K	320.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	338.10	J/mol×K	320.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	345.20	J/mol×K	325.00	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	343.40	J/mol×K	325.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	380.70	J/mol×K	380.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	348.40	J/mol×K	330.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	354.90	J/mol×K	335.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	353.00	J/mol×K	335.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	359.10	J/mol×K	340.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	357.20	J/mol×K	340.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	363.20	J/mol×K	345.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	361.50	J/mol×K	345.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	367.30	J/mol×K	350.01	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	365.80	J/mol×K	350.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	370.90	J/mol×K	355.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	369.40	J/mol×K	355.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	373.90	J/mol×K	360.00	Calorimetric and FTIR study of selected aliphatic heptanols

cpl	372.30	J/mol×K	360.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	376.30	J/mol×K	365.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	374.80	J/mol×K	365.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	378.10	J/mol×K	370.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	376.60	J/mol×K	370.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	379.60	J/mol×K	375.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	378.20	J/mol×K	375.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	379.50	J/mol×K	380.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	350.30	J/mol×K	330.00	Calorimetric and FTIR study of selected aliphatic heptanols
cpl	381.10	J/mol×K	382.85	Calorimetric and FTIR study of selected aliphatic heptanols
dvisc	0.1594974	Pa×s	214.47	Joback Method
dvisc	0.0221021	Pa×s	253.94	Joback Method
dvisc	0.0052125	Pa×s	293.41	Joback Method
dvisc	0.0007266	Pa×s	372.36	Joback Method
dvisc	0.0003601	Pa×s	411.83	Joback Method
dvisc	0.0002018	Pa×s	451.30	Joback Method
dvisc	0.0017316	Pa×s	332.88	Joback Method
hvapt	59.20	kJ/mol	378.50	NIST Webbook
hvapt	67.00	kJ/mol	288.50	NIST Webbook
hvapt	60.30	kJ/mol	377.50	NIST Webbook
hvapt	64.70	kJ/mol	279.00	NIST Webbook
hvapt	53.10	kJ/mol	389.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	339.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54409e+01
Coeff. B	-3.32014e+03
Coeff. C	-1.18372e+02
Temperature range (K), min.	337.47
Temperature range (K), max.	446.14

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C589822&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
hfl:	Liquid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
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