3-Pentanol, 3-ethyl-

Other names:	3-Aethyl-pentanol-(3)
	3-Ethyl-3-hydroxypentane
	3-Ethyl-3-pentanol
	3-ethylpentan-3-ol
	Ethyl-3 pentanol-3
	Triethylcarbinol
	Triethylmethanol
Inchi:	InChI=1S/C7H16O/c1-4-7(8,5-2)6-3/h8H,4-6H2,1-3H3
InchiKey:	XKIRHOWVQWCYBT-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCC(O)(CC)CC
Mol. weight [g/mol]:	116.20
CAS:	597-49-9

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	57.30 ± 0.20	kJ/mol	NIST Webbook
log10ws	-0.85		Estimated Solubility Method
log10ws	-0.85		Aqueous Solubility Prediction Method
logp	1.948		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
rinpol	866.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	853.00		NIST Webbook

rinpol	853.00		NIST Webbook
rinpol	853.00		NIST Webbook
ripol	1183.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1212.00		NIST Webbook
ripol	1208.00		NIST Webbook
ripol	1205.00		NIST Webbook
ripol	1183.00		NIST Webbook
tb	448.51	K	Joback Method
tc	618.48	K	Joback Method
tf	259.40	K	Calorimetric and FTIR study of selected aliphatic heptanols
tf	260.40	K	Aqueous Solubility Prediction Method
tf	260.81 ± 0.20	K	NIST Webbook
tf	258.95 ± 0.50	K	NIST Webbook
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	353.91	J/mol×K	298.15	NIST Webbook
dvisc	0.0003910	Pa×s	412.41	Joback Method
dvisc	0.0007730	Pa×s	376.30	Joback Method
dvisc	0.0017661	Pa×s	340.20	Joback Method
dvisc	0.0049095	Pa×s	304.10	Joback Method
dvisc	0.0179763	Pa×s	267.99	Joback Method
dvisc	0.0002207	Pa×s	448.51	Joback Method
dvisc	0.0985996	Pa×s	231.89	Joback Method
hvapt	55.20	kJ/mol	362.00	NIST Webbook
hvapt	51.30	kJ/mol	362.50	NIST Webbook

pvap	0.20	kPa	290.30	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	302.20	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	0.66	kPa	305.20	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	0.81	kPa	308.20	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	1.01	kPa	311.20	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	0.16	kPa	287.30	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	0.12	kPa	284.30	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	0.09	kPa	281.30	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	278.40	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	0.05	kPa	275.30	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	0.41	kPa	299.30	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	0.32	kPa	296.30	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	0.26	kPa	293.30	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	414.20	K	99.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58447e+01
Coeff. B	-3.95755e+03
Coeff. C	-6.24770e+01
Temperature range (K), min.	316.87
Temperature range (K), max.	438.20

Datasets

Speed of sound, m/s

Temperature, K - Liquid	Pressure, kPa - Liquid	Speed of sound, m/s - Liquid
303.15	100.00	1269.7

303.15	10000.00	1326.5
303.15	20000.00	1379.5
303.15	30000.00	1429.1
303.15	40000.00	1474.3
303.15	50000.00	1515.9
303.15	60000.00	1556.7
303.15	70000.00	1594.7
303.15	80000.00	1632.3
303.15	90000.00	1667.3
303.15	100000.00	1700.2
313.15	100.00	1229.3
313.15	10000.00	1289.3
313.15	20000.00	1346.0
313.15	30000.00	1393.8
313.15	40000.00	1440.8
313.15	50000.00	1484.5
313.15	60000.00	1526.0
313.15	70000.00	1564.6
313.15	80000.00	1602.2
313.15	90000.00	1638.3
313.15	100000.00	1672.4
323.15	100.00	1189.8
323.15	10000.00	1255.2
323.15	20000.00	1311.9
323.15	30000.00	1364.3
323.15	40000.00	1412.8
323.15	50000.00	1459.0
323.15	60000.00	1500.7
323.15	70000.00	1541.0
323.15	80000.00	1580.4
323.15	90000.00	1616.9
323.15	100000.00	1651.3
333.15	100.00	1152.4
333.15	10000.00	1217.3
333.15	20000.00	1277.4
333.15	30000.00	1330.3
333.15	40000.00	1379.9
333.15	50000.00	1426.5
333.15	60000.00	1470.6
333.15	70000.00	1511.0
333.15	80000.00	1550.1
333.15	90000.00	1587.4
333.15	100000.00	1622.8
343.15	100.00	1113.0

343.15	10000.00	1180.3
343.15	20000.00	1241.1
343.15	30000.00	1297.2
343.15	40000.00	1349.5
343.15	50000.00	1396.0
343.15	60000.00	1441.1
343.15	70000.00	1482.7
343.15	80000.00	1522.0
343.15	90000.00	1560.4
343.15	100000.00	1596.4
353.15	100.00	1073.7
353.15	10000.00	1144.0
353.15	20000.00	1207.5
353.15	30000.00	1264.4
353.15	40000.00	1317.4
353.15	50000.00	1366.0
353.15	60000.00	1411.1
353.15	70000.00	1454.8
353.15	80000.00	1494.6
353.15	90000.00	1533.6
353.15	100000.00	1570.4
363.15	100.00	1034.6
363.15	10000.00	1107.3
363.15	20000.00	1172.7
363.15	30000.00	1232.5
363.15	40000.00	1286.4
363.15	50000.00	1336.4
363.15	60000.00	1383.4
363.15	70000.00	1427.4
363.15	80000.00	1467.9
363.15	90000.00	1507.1
363.15	100000.00	1544.3
373.15	100.00	994.7
373.15	10000.00	1072.0
373.15	20000.00	1139.6
373.15	30000.00	1200.6
373.15	40000.00	1256.3
373.15	50000.00	1307.4
373.15	60000.00	1354.2
373.15	70000.00	1400.0
373.15	80000.00	1440.9
373.15	90000.00	1481.4
373.15	100000.00	1519.4

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Study of the volumetric properties of weakly associated alcohols by means of high pressure speed of sound measurements:	https://www.doi.org/10.1016/j.jct.2005.10.002
Calorimetric and FTIR study of selected aliphatic heptanols:	https://www.doi.org/10.1016/j.fluid.2016.04.003
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Effect of Isomerism on the Liquid-Liquid Phase Behavior of Mixtures of 1-Alkyl-3-methylimidazolium Bis((trifluoromethyl)sulfonyl)amide Ionic Liquids with Heptanol:	https://www.doi.org/10.1021/acs.jced.8b01203
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C597499&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume