3-Hexanol

Other names:	3-hydroxyhexane
	C2H5CH(OH)C3H7
	Ethylpropylcarbinol
	Hexan-3-ol
	Hexanol-(3)
	ethyl propyl carbinol
Inchi:	InChI=1S/C6H14O/c1-3-5-6(7)4-2/h6-7H,3-5H2,1-2H3
InchiKey:	ZOCHHNOQQHDWHG-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CCCC(O)CC
Mol. weight [g/mol]:	102.17
CAS:	623-37-0

Physical Properties

Property code	Value	Unit	Source
gf	-139.62	kJ/mol	Joback Method
hf	-332.80 ± 2.20	kJ/mol	NIST Webbook
hfl	-390.30 ± 0.88	kJ/mol	NIST Webbook
hfus	11.86	kJ/mol	Joback Method
hvap	58.60 ± 0.40	kJ/mol	NIST Webbook
ie	10.15	eV	NIST Webbook
ie	9.63 ± 0.03	eV	NIST Webbook
log10ws	-0.80		Aqueous Solubility Prediction Method
log10ws	-0.80		Estimated Solubility Method
logp	1.557		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3360.00 ± 50.00	kPa	NIST Webbook
pc	3360.00 ± 20.00	kPa	NIST Webbook
rhoc	266.68 ± 6.13	kg/m3	NIST Webbook
rhoc	266.68 ± 2.04	kg/m3	NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	801.30		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	797.00		NIST Webbook

rinpol	785.00	NIST Webbook
rinpol	797.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	793.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	762.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	790.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	801.30	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	780.20	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	797.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	783.80	NIST Webbook
rinpol	782.60	NIST Webbook
rinpol	778.50	NIST Webbook
rinpol	774.80	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	780.20	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	784.00	NIST Webbook
ripol	1180.00	NIST Webbook
ripol	1211.00	NIST Webbook

ripol	1207.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1211.00		NIST Webbook
ripol	1211.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1189.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1202.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1222.00		NIST Webbook
ripol	1206.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1184.00		NIST Webbook
ripol	1198.00		NIST Webbook
ripol	1222.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1189.00		NIST Webbook
tb	408.75 ± 0.50	K	NIST Webbook
tb	407.90 ± 1.00	K	NIST Webbook
tb	408.20	K	NIST Webbook
tb	406.15 ± 2.00	K	NIST Webbook
tb	407.40 ± 1.50	K	NIST Webbook
tb	406.65 ± 2.00	K	NIST Webbook
tb	408.15 ± 2.00	K	NIST Webbook
tb	408.15 ± 2.00	K	NIST Webbook
tb	408.15 ± 2.00	K	NIST Webbook
tb	408.65 ± 1.00	K	NIST Webbook
tb	406.65 ± 2.00	K	NIST Webbook
tb	406.15 ± 2.00	K	NIST Webbook
tb	408.65 ± 2.00	K	NIST Webbook
tb	409.00 ± 3.00	K	NIST Webbook
tb	407.15 ± 2.00	K	NIST Webbook
tb	408.67 ± 0.20	K	NIST Webbook
tb	406.65 ± 2.00	K	NIST Webbook
tb	408.00 ± 6.00	K	NIST Webbook

tb	407.15 ± 2.00	K	NIST Webbook
tb	407.15 ± 2.00	K	NIST Webbook
tb	388.55 ± 0.40	K	NIST Webbook
tb	404.15 ± 3.00	K	NIST Webbook
tb	406.15 ± 2.00	K	NIST Webbook
tc	582.20 ± 0.80	K	NIST Webbook
tc	582.40 ± 0.50	K	NIST Webbook
tc	582.58	K	NIST Webbook
tc	582.48 ± 0.30	K	NIST Webbook
tf	203.20	K	Joback Method
vc	0.383	m3/kmol	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.74	J/mol×K	428.42	Joback Method
cpg	226.97	J/mol×K	483.27	Joback Method
cpg	236.05	J/mol×K	510.70	Joback Method
cpg	244.78	J/mol×K	538.12	Joback Method
cpg	253.18	J/mol×K	565.55	Joback Method
cpg	261.25	J/mol×K	592.97	Joback Method
cpg	217.54	J/mol×K	455.85	Joback Method
cpl	269.27	J/mol×K	298.15	NIST Webbook
cpl	286.20	J/mol×K	298.00	NIST Webbook
dvisc	0.0035200	Pa×s	303.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
dvisc	0.0023400	Pa×s	313.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
dvisc	0.0015800	Pa×s	323.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
hvapt	46.10	kJ/mol	382.00	NIST Webbook
hvapt	57.50	kJ/mol	300.00	NIST Webbook

hvapt	51.50	kJ/mol	371.00	NIST Webbook
hvapt	57.40	kJ/mol	298.00	NIST Webbook
hvapt	46.40	kJ/mol	353.00	NIST Webbook
pvap	1.36	kPa	316.48	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	1.14	kPa	313.79	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.92	kPa	310.61	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.75	kPa	307.60	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.55	kPa	303.49	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	0.41	kPa	299.62	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.35	kPa	297.37	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.26	kPa	293.48	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.25	kPa	293.36	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.12	kPa	284.32	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	0.11	kPa	283.54	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.09	kPa	280.41	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	1.00	kPa	311.78	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.69	kPa	306.58	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.37	kPa	298.18	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	0.17	kPa	288.55	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.08	kPa	280.21	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52054e+01
Coeff. B	-3.58018e+03
Coeff. C	-6.88330e+01
Temperature range (K), min.	308.83
Temperature range (K), max.	430.69

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems:	https://www.doi.org/10.1021/je0498053
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623370&Units=SI
Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols:	https://www.doi.org/10.1021/acs.jced.6b00576

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

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