Acetic acid, hexyl ester

Other names:	1-HEXYL ACETATE
	Acetic acid n-hexyl ester
	FEMA No. 2565
	Hexyl acetate
	Hexyl alcohol, acetate
	Hexyl ester of acetic acid
	Hexyl ethanoate
	Hexylester kyseliny octove
	N-HEXYL ACETATE
	N-HEXYL ETHANOATE
	NSC 7323
	ethanoic acid, hexyl ester
Inchi:	InChI=1S/C8H16O2/c1-3-4-5-6-7-10-8(2)9/h3-7H2,1-2H3
InchiKey:	AOGQPLXWSUTHQB-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCCCCOC(C)=O
Mol. weight [g/mol]:	144.21
CAS:	142-92-7

Physical Properties

Property code	Value	Unit	Source
gf	-217.44	kJ/mol	Joback Method
hf	-453.25	kJ/mol	Joback Method
hfus	19.26	kJ/mol	Joback Method
hvap	52.10	kJ/mol	NIST Webbook
hvap	51.90 ± 0.30	kJ/mol	NIST Webbook
log10ws	-2.46		Aqueous Solubility Prediction Method
logp	2.130		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=1)		KDB
pc	2657.03	kPa	Joback Method
rinpol	995.00		NIST Webbook
rinpol	1008.70		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1008.00		NIST Webbook

rinpol	993.00	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	990.60	NIST Webbook
rinpol	991.10	NIST Webbook
rinpol	988.00	NIST Webbook
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tb	444.63	K	KDB
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tb	442.20	K	NIST Webbook
tb	442.00	K	NIST Webbook
tb	464.00 ± 2.00	K	NIST Webbook
tb	442.40 ± 1.50	K	NIST Webbook
tb	429.15 ± 3.00	K	NIST Webbook
tb	444.63 ± 0.30	K	NIST Webbook
tb	441.00 ± 4.00	K	NIST Webbook
tc	633.80	K	Joback Method
tf	212.25	K	KDB
tf	192.85	K	Aqueous Solubility Prediction Method
tf	212.10 ± 0.05	K	NIST Webbook
tf	192.30 ± 0.50	K	NIST Webbook
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.77	J/mol×K	633.80	Joback Method

cpg	279.70	J/mol×K	458.73	Joback Method
cpg	291.94	J/mol×K	487.91	Joback Method
cpg	303.75	J/mol×K	517.09	Joback Method
cpg	326.10	J/mol×K	575.44	Joback Method
cpg	336.64	J/mol×K	604.62	Joback Method
cpg	315.14	J/mol×K	546.26	Joback Method
dvisc	0.0007820	Pa×s	318.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0009620	Pa×s	303.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0011180	Pa×s	293.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0007330	Pa×s	323.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005790	Pa×s	343.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006890	Pa×s	328.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006490	Pa×s	333.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006120	Pa×s	338.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008360	Pa×s	313.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

dvisc	0.0010360	Pa×s	298.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008950	Pa×s	308.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
hfust	19.83	kJ/mol	212.10	NIST Webbook
hfust	19.83	kJ/mol	212.10	NIST Webbook
hvapt	46.20	kJ/mol	418.50	NIST Webbook
hvapt	48.90	kJ/mol	342.50	NIST Webbook
hvapt	50.90	kJ/mol	373.50	NIST Webbook
pvap	55.00	kPa	422.59	Phase Equlibria for Hexyl Acetate Reactive Distillation
pvap	50.00	kPa	419.47	Phase Equlibria for Hexyl Acetate Reactive Distillation
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pvap	90.00	kPa	439.98	Phase Equlibria for Hexyl Acetate Reactive Distillation
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pvap	25.00	kPa	397.97	Phase Equlibria for Hexyl Acetate Reactive Distillation
pvap	0.33	kPa	309.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.27	kPa	306.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.23	kPa	303.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
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pvap	0.15	kPa	297.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
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pvap	0.10	kPa	291.90	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

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pvap	0.03	kPa	274.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.03	kPa	277.70	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	75.00	kPa	433.38	Phase Equlibria for Hexyl Acetate Reactive Distillation
pvap	0.04	kPa	280.80	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
rfi	1.40960		293.15	Liquid-liquid equilibria study of the (water + phosphoric acid + hexyl or cyclohexyl acetate) systems at T = (298.15, 308.15, and 318.15) K: Measurement and thermodynamic modelling

rhol	855.00	kg/m3	313.15	Densities, Viscosities, and Sound Speed of Binary Mixtures of Hexyl Acetate with Tetrahydrofuran, 1,4-Dioxane, Anisole, and Butyl Vinyl Ether	
rhol	859.80	kg/m3	308.15	Densities, Viscosities, and Sound Speed of Binary Mixtures of Hexyl Acetate with Tetrahydrofuran, 1,4-Dioxane, Anisole, and Butyl Vinyl Ether	
rhol	863.90	kg/m3	303.15	Densities, Viscosities, and Sound Speed of Binary Mixtures of Hexyl Acetate with Tetrahydrofuran, 1,4-Dioxane, Anisole, and Butyl Vinyl Ether	
rhol	868.30	kg/m3	298.15	Densities, Viscosities, and Sound Speed of Binary Mixtures of Hexyl Acetate with Tetrahydrofuran, 1,4-Dioxane, Anisole, and Butyl Vinyl Ether	
rhol	868.52	kg/m3	298.15	Experimental and theoretical study of surface tension of binary mixtures of (n-alkyl acetates + heptane, benzene, and toluene)	
rhol	868.52	kg/m3	298.15	Surface Tension and Surface Properties of Binary Mixtures of 1,4-Dioxane or N,N-Dimethyl Formamide with n-Alkyl Acetates	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54294e+01
Coeff. B	-4.08917e+03
Coeff. C	-6.47630e+01
Temperature range (K), min.	334.82
Temperature range (K), max.	468.91

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.03443e+01
Coeff. B	-8.74286e+03
Coeff. C	-9.31977e+00
Coeff. D	3.93049e-06
Temperature range (K), min.	192.25
Temperature range (K), max.	618.00

Sources

Liquid-liquid equilibria study of the (water + phosphoric acid + hexyl or cyclohexyl acetate) systems at T = (298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1016/j.jct.2016.03.025
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Experimental and theoretical study of surface tension of binary mixtures of (n-alkyl acetates + heptane, benzene, and toluene):	https://www.doi.org/10.1016/j.jct.2008.10.009
Measurement and thermodynamic modelling.	
Yaws Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C142927&Units=SI
Surface Tension and Surface Properties of Binary Mixtures of 1,4-Dioxane or N,N-Dimethyl Formamide with n-Alkyl Acetates:	https://www.doi.org/10.1021/je9002114
Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates:	https://www.doi.org/10.1016/j.jct.2005.08.003
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1107
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Densities, Viscosities, and Sound Speed of Binary Mixtures of Hexyl Acetate with Tetrahydrofuran, 1,4-Dioxane, Anisole, and Butyl Vinyl Ether:	https://www.doi.org/10.1021/je400539h
Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters:	https://www.doi.org/10.1021/je050001c
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1107
Phase Equlibria for Hexyl Acetate Reactive Distillation:	https://www.doi.org/10.1021/je050141m

Legend

cpg:	Ideal gas 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
hfust:	Enthalpy of fusion at a given temperature
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid 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