Acetic acid, heptyl ester

Other names:	1-HEPTYL ACETATE
	Acetate C-7
	Acetic acid n-heptyl ester
	HEPTANYL ACETATE
	Heptanol acetate
	Heptyl acetate
	N-HEPTYL ETHANOATE
	heptyl ethanoate
	n-Heptyl acetate
Inchi:	InChI=1S/C9H18O2/c1-3-4-5-6-7-8-11-9(2)10/h3-8H2,1-2H3
InchiKey:	ZCZSIDMEHXZRLG-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCCCCOC(C)=O
Mol. weight [g/mol]:	158.24
CAS:	112-06-1

Physical Properties

Property code	Value	Unit	Source
gf	-209.02	kJ/mol	Joback Method
hf	-473.89	kJ/mol	Joback Method
hfus	21.85	kJ/mol	Joback Method
hvap	57.10 ± 0.20	kJ/mol	NIST Webbook
hvap	56.90	kJ/mol	NIST Webbook
log10ws	-2.45		Crippen Method
logp	2.520		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1112.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1089.15		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1091.00		NIST Webbook

rinpol	1095.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1118.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1112.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1091.70	NIST Webbook
rinpol	1089.15	NIST Webbook
rinpol	1110.21	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1070.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1070.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1083.00	NIST Webbook
rinpol	1083.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1096.00	NIST Webbook

rinpol	1095.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1111.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1370.00		NIST Webbook
ripol	1361.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1385.00		NIST Webbook
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ripol	1385.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1377.00		NIST Webbook
ripol	1401.00		NIST Webbook
tb	464.50 ± 1.50	K	NIST Webbook
tb	465.60 ± 0.30	K	NIST Webbook
tb	464.00 ± 3.00	K	NIST Webbook
tb	465.60	K	KDB
tb	501.00 ± 3.00	K	NIST Webbook
tc	655.29	K	Joback Method
tf	223.00 ± 0.50	K	NIST Webbook
tf	222.95	K	KDB

vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.29	J/mol×K	655.29	Joback Method
cpg	336.15	J/mol×K	510.56	Joback Method
cpg	348.92	J/mol×K	539.50	Joback Method
cpg	361.21	J/mol×K	568.45	Joback Method
cpg	373.04	J/mol×K	597.40	Joback Method
cpg	384.40	J/mol×K	626.35	Joback Method
cpg	322.89	J/mol×K	481.61	Joback Method
dvisc	0.0033103	Pa×s	263.35	Joback Method
dvisc	0.0016384	Pa×s	299.73	Joback Method
dvisc	0.0009442	Pa×s	336.10	Joback Method
dvisc	0.0006060	Pa×s	372.48	Joback Method
dvisc	0.0004209	Pa×s	408.86	Joback Method
dvisc	0.0003103	Pa×s	445.23	Joback Method
dvisc	0.0002395	Pa×s	481.61	Joback Method
hvapt	49.20	kJ/mol	432.50	NIST Webbook
pvap	7.04e-03	kPa	274.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.10	kPa	306.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.08	kPa	303.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.06	kPa	300.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

pvap	0.05	kPa	297.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.04	kPa	294.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.03	kPa	290.90	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.02	kPa	287.90	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.02	kPa	284.80	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.01	kPa	281.80	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.01	kPa	278.70	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	8.51e-03	kPa	276.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

rhol	870.58	kg/m3	293.20	Liquid-liquid equilibrium data for ternary systems of water + acetic acid + acetate esters at 293.2 K and 303.2 K and ~ 95 kPa
rhol	852.59	kg/m3	313.20	Liquid-liquid equilibrium data for ternary systems of water + acetic acid + acetate esters at 293.2 K and 303.2 K and ~ 95 kPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54381e+01
Coeff. B	-4.25680e+03
Coeff. C	-7.05730e+01
Temperature range (K), min.	351.54
Temperature range (K), max.	490.93

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.29169e+02
Coeff. B	-1.14540e+04
Coeff. C	-1.65742e+01
Coeff. D	8.63888e-06
Temperature range (K), min.	387.15
Temperature range (K), max.	478.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C112061&Units=SI

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1116.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Liquid-liquid equilibrium data for ternary systems of water + acetic acid + acetate esters at 293.2 K and 303.2 K and ~ 95 kPa:	https://www.doi.org/10.1016/j.fluid.2018.02.003
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=1116
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
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

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