2-Hexen-1-ol, acetate, (E)-

Other names:	(E)-2-Hexen-1-yl acetate
	(E)-2-Hexenyl acetate
	(E)-Hex-2-enyl acetate
	2-Hexen-1-ol acetate
	2-Hexen-1-yl acetate
	2-Hexen-1-yl-acetate, (E)-
	2-Hexenyl acetate
	2-Hexenyl acetate, trans-
	Hex-2-enyl acetate, trans-
	hex-2-en-1-yl acetate
	hex-2-enyl acetate
	trans-2-Hexenyl acetate
	trans-Hex-2-enyl acetate
Inchi:	InChI=1S/C8H14O2/c1-3-4-5-6-7-10-8(2)9/h5-6H,3-4,7H2,1-2H3/b6-5+
InchiKey:	HRHOWZHRCRZVCU-AATRIKPKSA-N
Formula:	C8H14O2
SMILES:	CCCC=CCOC(C)=O
Mol. weight [g/mol]:	142.20
CAS:	2497-18-9

Physical Properties

Property code	Value	Unit	Source
gf	-137.22	kJ/mol	Joback Method
hf	-336.03	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	42.52	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.906		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
rinpol	995.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	995.00		NIST Webbook

rinpol	994.00	NIST Webbook
rinpol	1018.00	NIST Webbook
rinpol	1028.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1020.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1014.00	NIST Webbook
rinpol	1019.00	NIST Webbook
rinpol	995.80	NIST Webbook
rinpol	1017.00	NIST Webbook
rinpol	1017.00	NIST Webbook
rinpol	997.00	NIST Webbook
rinpol	997.00	NIST Webbook
rinpol	996.00	NIST Webbook
rinpol	997.00	NIST Webbook
rinpol	994.00	NIST Webbook
rinpol	997.00	NIST Webbook
rinpol	991.00	NIST Webbook
rinpol	991.40	NIST Webbook
rinpol	1010.00	NIST Webbook
ripol	1333.00	NIST Webbook
ripol	1322.00	NIST Webbook
ripol	1325.00	NIST Webbook
ripol	1333.00	NIST Webbook
ripol	1331.00	NIST Webbook
ripol	1322.00	NIST Webbook
ripol	1325.00	NIST Webbook
ripol	1337.00	NIST Webbook
ripol	1337.00	NIST Webbook
ripol	1342.00	NIST Webbook
ripol	1341.00	NIST Webbook
ripol	1331.00	NIST Webbook
ripol	1323.00	NIST Webbook
ripol	1338.00	NIST Webbook
ripol	1344.00	NIST Webbook
ripol	1346.00	NIST Webbook
ripol	1315.00	NIST Webbook
ripol	1334.00	NIST Webbook
ripol	1320.00	NIST Webbook
ripol	1321.00	NIST Webbook
ripol	1333.00	NIST Webbook
ripol	1354.00	NIST Webbook
ripol	1340.00	NIST Webbook
ripol	1323.00	NIST Webbook

ripol	1346.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1337.00		NIST Webbook
ripol	1344.00		NIST Webbook
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ripol	1322.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1359.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1323.00		NIST Webbook
tb	438.00	K	NIST Webbook
tb	438.70	K	NIST Webbook
tc	646.21	K	Joback Method
tf	247.00	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.49	J/mol×K	646.21	Joback Method
cpg	317.95	J/mol×K	615.66	Joback Method
cpg	307.96	J/mol×K	585.10	Joback Method
cpg	297.52	J/mol×K	554.55	Joback Method
cpg	286.60	J/mol×K	524.00	Joback Method
cpg	275.19	J/mol×K	493.44	Joback Method
cpg	263.30	J/mol×K	462.89	Joback Method

dvisc	0.0009010	Pa×s	293.15	Density and Viscosity for a Binary Mixture of cis-3-Hexenyl Formate, Butyl Acetate, trans-2-Hexenyl Acetate, and cis-3-Hexenyl Acetate with Ethanol at Several Temperatures	
dvisc	0.0005140	Pa×s	333.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0005470	Pa×s	328.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0007700	Pa×s	303.15	Density and Viscosity for a Binary Mixture of cis-3-Hexenyl Formate, Butyl Acetate, trans-2-Hexenyl Acetate, and cis-3-Hexenyl Acetate with Ethanol at Several Temperatures	
dvisc	0.0006660	Pa×s	313.15	Density and Viscosity for a Binary Mixture of cis-3-Hexenyl Formate, Butyl Acetate, trans-2-Hexenyl Acetate, and cis-3-Hexenyl Acetate with Ethanol at Several Temperatures	
dvisc	0.0005820	Pa×s	323.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0006220	Pa×s	318.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	

dvisc	0.0006660	Pa×s	313.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0007150	Pa×s	308.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0007700	Pa×s	303.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008310	Pa×s	298.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0009010	Pa×s	293.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50611e+01
Coeff. B	-3.96667e+03
Coeff. C	-6.30810e+01
Temperature range (K), min.	331.58
Temperature range (K), max.	469.94

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters:	https://www.doi.org/10.1021/je050001c

Density and Viscosity for a Binary Mixture of cis-3-Hexenyl Formate, Butyl Acetate, trans-2-Hexenyl Acetate, and cis-3-Hexenyl Acetate with Ethanol at Several Temperatures:	https://www.doi.org/10.1021/je0500025
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2497189&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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