3-Hexen-1-ol, acetate, (Z)-

Other names:	(3Z)-3-Hexenyl acetate
	(Z)-3-Hexen-1-ol acetate
	(Z)-3-Hexen-1-yl, acetate
	(Z)-3-Hexenol acetate
	(Z)-3-hexenyl acetate
	(Z)-Hex-3-enyl acetate
	3(Z)-Hexenyl acetate
	3-Hexenol acetate, cis
	Acetic acid cis-3-hexenyl ester
	Hex-3(Z)-enyl acetate
	Z-Hex-3-en-1-yl acetate
	cis-3-Hexen-1-ol, acetate
	cis-3-Hexenyl Acetate
	cis-3-Hexenyl-1-acetate
	cis-Hex-3-enyl acetate
Inchi:	InChI=1S/C8H14O2/c1-3-4-5-6-7-10-8(2)9/h4-5H,3,6-7H2,1-2H3/b5-4-
InchiKey:	NPFVOOAXDOBMCE-PLNGDYQASA-N
Formula:	C8H14O2
SMILES:	CCC=CCCOC(C)=O
Mol. weight [g/mol]:	142.20
CAS:	3681-71-8

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	996.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	996.00		NIST Webbook

rinpol	996.00	NIST Webbook
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ripol	1312.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1315.00		NIST Webbook
tb	442.00	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	263.30	J/mol×K	462.89	Joback Method
cpg	275.19	J/mol×K	493.44	Joback Method
cpg	286.60	J/mol×K	524.00	Joback Method
cpg	297.52	J/mol×K	554.55	Joback Method
cpg	307.96	J/mol×K	585.10	Joback Method
cpg	317.95	J/mol×K	615.66	Joback Method
cpg	327.49	J/mol×K	646.21	Joback Method
dvisc	0.0007630	Pa×s	303.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008230	Pa×s	298.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008930	Pa×s	293.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0007080	Pa×s	308.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006600	Pa×s	313.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006160	Pa×s	318.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005760	Pa×s	323.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

dvisc	0.0005420	Pa×s	328.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005090	Pa×s	333.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008930	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	0.0007630	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	0.0006600	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

Sources

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NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3681718&Units=SI

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
Green Leaf Volatiles on Aqueous Air/Water Interfaces: A Combined Experimental and Molecular Simulation Study:	https://www.doi.org/10.1021/je500114m

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
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