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: $C_8H_{14}O_2$

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	1007.00		NIST Webbook
rinpol	987.00		NIST Webbook
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ripol	1308.00		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

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 Atmospheric Air/Water Interfaces: A Combined Experimental and Molecular Simulation Study: https://www.doi.org/10.1021/je500114m

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=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

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

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