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

Other names:	(3E)-Hexenyl acetate
	(E)-3-Hexen-1-ol acetate
	(E)-3-Hexen-1-yl acetate
	(E)-3-Hexenol acetate
	(E)-3-Hexenyl acetate
	(E)-Hex-3-enol acetate
	trans-3-Hexen-1-ol, acetate
	trans-3-Hexenyl acetate
	(3E)-3-Hexenyl acetate
	(E)-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-SNAWJCMRSA-N
Formula:	C8H14O2
SMILES:	CCC=CCCOC(C)=O
Mol. weight [g/mol]:	142.20
CAS:	3681-82-1

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	1005.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	996.40		NIST Webbook
rinpol	967.00		NIST Webbook

rinpol	1002.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	983.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1298.00		NIST Webbook
ripol	1298.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1350.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1306.00		NIST Webbook
ripol	1300.00		NIST Webbook
tb	462.89	K	Joback Method
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	0.0030324	Pa×s	247.00	Joback Method
dvisc	0.0014687	Pa×s	282.98	Joback Method
dvisc	0.0008378	Pa×s	318.96	Joback Method
dvisc	0.0005355	Pa×s	354.94	Joback Method
dvisc	0.0003717	Pa×s	390.93	Joback Method
dvisc	0.0002744	Pa×s	426.91	Joback Method
dvisc	0.0002123	Pa×s	462.89	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3681821&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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