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

Other names:	(3Z)-3-Hexenyl formate
	(Z)-3-Hexenyl format
	(Z)-3-Hexenyl formate
	(Z)-Hex-3-enyl formate
	cis-3-Hexen-1-ol formate
	cis-3-Hexenyl formate
	cis-«beta»-Hexenyl formate
	cis-Â«betaÂ»-Hexenyl formate
	«beta»,«gamma»-Hexenyl methanoate
	Â«betaÂ»,Â«gammaÂ»-Hexenyl methanoate
Inchi:	InChI=1S/C7H12O2/c1-2-3-4-5-6-9-7-8/h3-4,7H,2,5-6H2,1H3/b4-3-
InchiKey:	XJHQVZQZUGLZLS-ARJAWSKDSA-N
Formula:	C7H12O2
SMILES:	CCC=CCCOC=O
Mol. weight [g/mol]:	128.17
CAS:	33467-73-1

Physical Properties

Property code	Value	Unit	Source
gf	-116.24	kJ/mol	Joback Method
hf	-288.39	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	40.26	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
rinpol	903.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	902.40		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	903.00		NIST Webbook

ripol	1252.00		NIST Webbook
ripol	1254.00		NIST Webbook
ripol	1258.00		NIST Webbook
ripol	1261.00		NIST Webbook
ripol	1252.00		NIST Webbook
ripol	1260.00		NIST Webbook
tb	434.80	K	Joback Method
tc	614.89	K	Joback Method
tf	227.80	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.30	J/mol×K	434.80	Joback Method
cpg	234.73	J/mol×K	464.82	Joback Method
cpg	244.75	J/mol×K	494.83	Joback Method
cpg	254.34	J/mol×K	524.85	Joback Method
cpg	263.54	J/mol×K	554.86	Joback Method
cpg	272.34	J/mol×K	584.88	Joback Method
cpg	280.76	J/mol×K	614.89	Joback Method
dvisc	0.0004960	Pa×s	308.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005610	Pa×s	298.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005270	Pa×s	303.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005990	Pa×s	293.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

dvisc	0.0004690	Pa×s	313.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0004430	Pa×s	318.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0004210	Pa×s	323.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0004000	Pa×s	328.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003800	Pa×s	333.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003630	Pa×s	338.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003460	Pa×s	343.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005990	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	0.0005270	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	0.0004690	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.89075e+01
Coeff. B	-5.07474e+03
Coeff. C	-6.56080e+01
Temperature range (K), min.	338.15
Temperature range (K), max.	438.86

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=C33467731&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