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

Other names:	(3Z)-3-Hexenyl propionate
	(Z)-3-Hexen-1-ol, propanoate
	(Z)-3-Hexenyl propanoate
	(Z)-3-Hexenyl propionate
	(Z)-Hex-3-enyl propionate
	3-Hexen-1-ol, propionate, (Z)-
	Propanoic acid, (Z)-3-hexenyl ester
	Propionic acid cis-3-hexenyl ester
	cis-3-Hexenyl n-propionate
	cis-3-Hexenyl propionate
	cis-3-hexenyl propanoate
	cis-hex-3-en-1-yl propanoate
	cis-«beta»-Hexenyl propionate
	cis-Â«betaÂ»-Hexenyl propionate
	«beta»,«gamma»-Hexenyl propanoate, cis
	Â«betaÂ»,Â«gammaÂ»-Hexenyl propanoate, cis
Inchi:	InChI=1S/C9H16O2/c1-3-5-6-7-8-11-9(10)4-2/h5-6H,3-4,7-8H2,1-2H3/b6-5-
InchiKey:	LGTLDEUQCOJGFP-WAYWQWQTSA-N
Formula:	C9H16O2
SMILES:	CCC=CCCOC(=O)CC
Mol. weight [g/mol]:	156.22
CAS:	33467-74-2

Physical Properties

Property code	Value	Unit	Source
gf	-128.80	kJ/mol	Joback Method
hf	-356.67	kJ/mol	Joback Method
hfus	22.05	kJ/mol	Joback Method
hvap	44.74	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	1066.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1075.00		NIST Webbook

rinpol	1105.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1074.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1391.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1391.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1380.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1370.00		NIST Webbook
ripol	1392.00		NIST Webbook
tb	485.77	K	Joback Method
tc	667.32	K	Joback Method
tf	258.27	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.62	J/mol×K	667.32	Joback Method
cpg	306.02	J/mol×K	485.77	Joback Method
cpg	318.93	J/mol×K	516.03	Joback Method
cpg	331.30	J/mol×K	546.29	Joback Method
cpg	343.15	J/mol×K	576.54	Joback Method
cpg	354.47	J/mol×K	606.80	Joback Method
cpg	365.29	J/mol×K	637.06	Joback Method
dvisc	0.0002011	Pa×s	485.77	Joback Method
dvisc	0.0030655	Pa×s	258.27	Joback Method
dvisc	0.0014558	Pa×s	296.19	Joback Method
dvisc	0.0008186	Pa×s	334.10	Joback Method
dvisc	0.0005177	Pa×s	372.02	Joback Method

dvisc	0.0003563	Pa×s	409.94	Joback Method
dvisc	0.0002612	Pa×s	447.85	Joback Method
hvapt	55.70	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67913e+01
Coeff. B	-4.75041e+03
Coeff. C	-7.33810e+01
Temperature range (K), min.	361.22
Temperature range (K), max.	487.19

Sources

Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2015.02.015
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=C33467742&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
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