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 propanoate
	cis-3-hexenyl propionate
	cis-hex-3-en-1-yl propanoate
	cis-«beta»-Hexenyl propionate
	«beta»,«gamma»-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:	CC/C=C\CCOC(=O)CC
Mol. weight [g/mol]:	156.23
CAS:	33467-74-2

Physical Properties

Property code	Value	Unit	Source
af	0.4699		Cheméo Relay (1.0)
gf	-128.80	kJ/mol	Joback Method
hf	-447.71	kJ/mol	Cheméo Relay (1.0)
hfus	22.06	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Cheméo Relay (1.0)
ie	9.18	eV	Cheméo Relay (1.0)
log10ws	-2.03		Cheméo Relay (1.0)
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	1079.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1071.00		NIST Webbook

rinpol	1105.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1085.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1391.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1380.00		NIST Webbook
ripol	1391.00		NIST Webbook
ripol	1370.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1390.00		NIST Webbook
tb	449.39	K	Cheméo Relay (1.0)
tc	635.58	K	Cheméo Relay (1.0)
tf	174.38	K	Cheméo Relay (1.0)
vc	0.516	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.29	J/mol×K	637.06	Joback Method
cpg	375.62	J/mol×K	667.32	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	306.02	J/mol×K	485.77	Joback Method
dvisc	0.0008186	Pa×s	334.10	Joback Method
dvisc	0.0014558	Pa×s	296.19	Joback Method
dvisc	0.0030655	Pa×s	258.27	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
dvisc	0.0002011	Pa×s	485.77	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33467742&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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