Hexanoic acid, 3-hexenyl ester, (Z)-

Other names:	(3Z)-3-Hexenyl hexanoate
	(Z)-3-Hexen-1-ol, hexanoate
	(Z)-3-Hexenyl hexanoate
	(Z)-hex-3-enyl hexanoate
	3-Hexen-1-ol hexanoate, cis
	3-Hexen-1-ol, hexanoate, (Z)-
	3-Hexenyl hexanoate, (Z)-
	Hexanoic acid, (3Z)-3-hexen-1-yl ester
	Hexanoic acid, (3Z)-3-hexenyl ester
	cis-3-Hexenyl caproate
	cis-3-Hexenyl hexanoate
	cis-3-Hexenyl hexoate
	cis-3-Hexenyl n-hexanoate
	cis-Hexanoic acid, 3-hexenyl ester
	n-Caproic acid cis-3-hexenyl ester
Inchi:	InChI=1S/C12H22O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h5,7H,3-4,6,8-11H2,1-2H3/b7-5
InchiKey:	RGACQXBDYBCJCY-ALCCZGGFSA-N
Formula:	C12H22O2
SMILES:	CCC=CCCOC(=O)CCCCC
Mol. weight [g/mol]:	198.30
CAS:	31501-11-8

Physical Properties

Property code	Value	Unit	Source
gf	-103.54	kJ/mol	Joback Method
hf	-418.59	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1333.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1362.00		NIST Webbook

rinpol	1386.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1355.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1647.00		NIST Webbook
ripol	1647.00		NIST Webbook
ripol	1662.00		NIST Webbook
ripol	1647.00		NIST Webbook
ripol	1662.00		NIST Webbook
ripol	1654.00		NIST Webbook
ripol	1662.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1646.00		NIST Webbook
ripol	1665.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1638.00		NIST Webbook
ripol	1662.00		NIST Webbook
ripol	1642.00		NIST Webbook
tb	554.41	K	Joback Method
tc	730.90	K	Joback Method
tf	292.08	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.74	J/mol×K	554.41	Joback Method
cpg	461.06	J/mol×K	583.82	Joback Method
cpg	475.72	J/mol×K	613.24	Joback Method
cpg	489.74	J/mol×K	642.65	Joback Method
cpg	503.13	J/mol×K	672.07	Joback Method
cpg	515.92	J/mol×K	701.48	Joback Method
cpg	528.11	J/mol×K	730.90	Joback Method
dvisc	0.0028734	Pa×s	292.08	Joback Method
dvisc	0.0012967	Pa×s	335.80	Joback Method
dvisc	0.0007029	Pa×s	379.52	Joback Method
dvisc	0.0004324	Pa×s	423.25	Joback Method
dvisc	0.0002914	Pa×s	466.97	Joback Method
dvisc	0.0002101	Pa×s	510.69	Joback Method
dvisc	0.0001595	Pa×s	554.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46081e+01
Coeff. B	-4.35803e+03
Coeff. C	-8.25320e+01
Temperature range (K), min.	386.85
Temperature range (K), max.	551.31

Sources

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

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=C31501118&Units=SI

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