Hexanoic acid, 2-propenyl ester

Other names:	2-Propenyl hexanoate
	2-Propenyl n-hexanoate
	Allyl caproate
	Allyl hexanoate
	Allyl n-hexanoate
	Allylester kyseliny kapronove
	Hexanoic acid, allyl ester
	allyl capronate
Inchi:	InChI=1S/C9H16O2/c1-3-5-6-7-9(10)11-8-4-2/h4H,2-3,5-8H2,1H3
InchiKey:	RCSBILYQLVXLJG-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	C=CCOC(=O)CCCCC
Mol. weight [g/mol]:	156.22
CAS:	123-68-2

Physical Properties

Property code	Value	Unit	Source
gf	-121.18	kJ/mol	Joback Method
hf	-348.46	kJ/mol	Joback Method
hfus	20.57	kJ/mol	Joback Method
hvap	44.11	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1065.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1065.00		NIST Webbook

rinpol	1057.00		NIST Webbook
rinpol	1057.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1370.00		NIST Webbook
tb	478.29	K	Joback Method
tc	655.34	K	Joback Method
tf	261.59	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.44	J/mol×K	478.29	Joback Method
cpg	318.12	J/mol×K	507.80	Joback Method
cpg	330.31	J/mol×K	537.31	Joback Method
cpg	342.00	J/mol×K	566.81	Joback Method
cpg	353.22	J/mol×K	596.32	Joback Method
cpg	363.97	J/mol×K	625.83	Joback Method
cpg	374.26	J/mol×K	655.34	Joback Method
dvisc	0.0030378	Pa×s	261.59	Joback Method
dvisc	0.0015428	Pa×s	297.71	Joback Method
dvisc	0.0009072	Pa×s	333.82	Joback Method
dvisc	0.0005918	Pa×s	369.94	Joback Method
dvisc	0.0004165	Pa×s	406.06	Joback Method
dvisc	0.0003104	Pa×s	442.17	Joback Method
dvisc	0.0002419	Pa×s	478.29	Joback Method
hvapt	55.20	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	1.50787e+01
Coeff. B	-4.13006e+03
Coeff. C	-6.87940e+01
Temperature range (K), min.	348.02
Temperature range (K), max.	491.64

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=C123682&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