Vinyl 2-ethylhexanoate

Other names:	2-Ethylhexanoic acid, vinyl ester
	2-Ethylhexoic acid, vinyl ester
	Hexanoic acid, 2-ethyl-, ethenyl ester
	Hexanoic acid, 2-ethyl-, vinyl ester
	Vinyl 2-ethylhexoate
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Inchi:	InChI=1S/C10H18O2/c1-4-7-8-9(5-2)10(11)12-6-3/h6,9H,3-5,7-8H2,1-2H3
InchiKey:	IGBZOHMCHDADGY-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=COC(=O)C(CC)CCCC
Mol. weight [g/mol]:	170.25
CAS:	94-04-2

Physical Properties

Property code	Value	Unit	Source
gf	-115.20	kJ/mol	Joback Method
hf	-374.38	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	45.95	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.889		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
tb	500.73	K	Joback Method
tc	679.83	K	Joback Method
tf	257.86	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.06	J/mol×K	500.73	Joback Method
cpg	364.01	J/mol×K	530.58	Joback Method
cpg	377.40	J/mol×K	560.43	Joback Method

cpg	390.22	J/mol×K	590.28	Joback Method
cpg	402.50	J/mol×K	620.13	Joback Method
cpg	414.23	J/mol×K	649.98	Joback Method
cpg	425.43	J/mol×K	679.83	Joback Method
dvisc	0.0042919	Pa×s	257.86	Joback Method
dvisc	0.0018562	Pa×s	298.34	Joback Method
dvisc	0.0009808	Pa×s	338.82	Joback Method
dvisc	0.0005939	Pa×s	379.29	Joback Method
dvisc	0.0003961	Pa×s	419.77	Joback Method
dvisc	0.0002837	Pa×s	460.25	Joback Method
dvisc	0.0002145	Pa×s	500.73	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32411e+01
Coeff. B	-3.58384e+03
Coeff. C	-6.74310e+01
Temperature range (K), min.	344.10
Temperature range (K), max.	519.38

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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume