Propanoic acid, ethenyl ester

Other names:	Propionic acid, vinyl ester
	Vinyl propanoate
	Vinyl propionate
	Vinylester kyseliny propionove
Inchi:	InChI=1S/C5H8O2/c1-3-5(6)7-4-2/h4H,2-3H2,1H3
InchiKey:	UIWXSTHGICQLQT-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	C=COC(=O)CC
Mol. weight [g/mol]:	100.12
CAS:	105-38-4

Physical Properties

Property code	Value	Unit	Source
gf	-154.86	kJ/mol	Joback Method
hf	-265.90	kJ/mol	Joback Method
hfus	10.21	kJ/mol	Joback Method
hvap	35.21	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.083		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	3857.88	kPa	Joback Method
rinpol	650.00		NIST Webbook
rinpol	669.00		NIST Webbook
rinpol	648.00		NIST Webbook
ripol	960.00		NIST Webbook
tb	386.77	K	Joback Method
tc	569.17	K	Joback Method
tf	216.51	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.35	J/mol×K	386.77	Joback Method
cpg	157.10	J/mol×K	417.17	Joback Method
cpg	164.59	J/mol×K	447.57	Joback Method
cpg	171.82	J/mol×K	477.97	Joback Method
cpg	178.80	J/mol×K	508.37	Joback Method
cpg	185.52	J/mol×K	538.77	Joback Method
cpg	191.98	J/mol×K	569.17	Joback Method
dvisc	0.0013568	Pa×s	244.89	Joback Method
dvisc	0.0024241	Pa×s	216.51	Joback Method
dvisc	0.0008567	Pa×s	273.26	Joback Method
dvisc	0.0005898	Pa×s	301.64	Joback Method
dvisc	0.0004330	Pa×s	330.02	Joback Method
dvisc	0.0003338	Pa×s	358.39	Joback Method
dvisc	0.0002673	Pa×s	386.77	Joback Method
rfi	1.40200		298.20	Ternary liquid liquid equilibria for mixtures of an ionic liquid + n-hexane + an organic compound involved in the kinetic resolution of rac-1-phenyl ethanol (rac-1-phenyl ethanol, vinyl propionate, rac-1-phenylethyl propionate or propionic acid) at 298.2K and atmospheric pressure
rfi	1.40153		298.15	Density, Refractive Index, Speed of Sound, and Vapor-Liquid Equilibria for Binary Mixtures of Methanol + Vinyl Propionate and Vinyl Acetate + Vinyl Propionate. Vapor Pressures of Vinyl Propionate

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30096e+01
Coeff. B	-2.24538e+03
Coeff. C	-1.03115e+02
Temperature range (K), min.	279.61
Temperature range (K), max.	394.79

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.69744e+01
Coeff. B	-7.22230e+03
Coeff. C	-9.01552e+00
Coeff. D	4.22805e-06
Temperature range (K), min.	293.15
Temperature range (K), max.	546.00

Sources

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=C105384&Units=SI
Density, Refractive Index, Speed of Sound, and Vapor-Liquid Equilibria for Binary Mixtures of Methanol + Vinyl Propionate and Vinyl Acetate + Vinyl Propionate. Vapor Pressures of Vinyl Propionate:	https://www.doi.org/10.1021/je049909d
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
Ternary liquid liquid equilibria for mixtures of an ionic liquid + n-hexane + an organic compound involved in the kinetic resolution of rac-1-phenyl ethanol (rac-1-phenyl ethanol, vinyl propionate, rac-1-phenylethyl propionate or propionic acid) at 298.2K and atmospheric pressure:	https://www.doi.org/10.1016/j.fluid.2007.10.011
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1172.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1172

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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
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