2-Propenoic acid, 2-propenyl ester

Other names:	Acrylic acid, allyl ester
	Allyl acrylate
	2-Propenyl ester of 2-propenoic acid
Inchi:	InChI=1S/C6H8O2/c1-3-5-8-6(7)4-2/h3-4H,1-2,5H2
InchiKey:	QTECDUFMBMSHKR-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	C=CCOC(=O)C=C
Mol. weight [g/mol]:	112.13
CAS:	999-55-3

Physical Properties

Property code	Value	Unit	Source
gf	-58.60	kJ/mol	Joback Method
hf	-161.11	kJ/mol	Joback Method
hfus	11.52	kJ/mol	Joback Method
hvap	36.77	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.902		Crippen Method
mcvol	94.240	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	734.00		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	742.00		NIST Webbook
tb	406.33	K	Joback Method
tc	591.53	K	Joback Method
tf	226.02	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.13	J/mol×K	406.33	Joback Method
cpg	209.20	J/mol×K	560.66	Joback Method
cpg	202.05	J/mol×K	529.79	Joback Method

cpg	194.57	J/mol×K	498.93	Joback Method
cpg	186.76	J/mol×K	468.06	Joback Method
cpg	178.62	J/mol×K	437.20	Joback Method
cpg	216.05	J/mol×K	591.53	Joback Method
dvisc	0.0002641	Pa×s	406.33	Joback Method
dvisc	0.0003287	Pa×s	376.28	Joback Method
dvisc	0.0004249	Pa×s	346.23	Joback Method
dvisc	0.0005768	Pa×s	316.18	Joback Method
dvisc	0.0008349	Pa×s	286.12	Joback Method
dvisc	0.0013182	Pa×s	256.07	Joback Method
dvisc	0.0023498	Pa×s	226.02	Joback Method

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=C999553&Units=SI
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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume