2-Propenoic acid, 2-methyl-, propyl ester

Other names:	Methacrylic acid, propyl ester
	Propyl 2-methyl-2-propenoate
	Propyl ester of 2-Methyl-2-propenoic acid
	Propyl methacrylate
	n-Propyl methacrylate
Inchi:	InChI=1S/C7H12O2/c1-4-5-9-7(8)6(2)3/h2,4-5H2,1,3H3
InchiKey:	NHARPDSAXCBDDR-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	C=C(C)C(=O)OCCC
Mol. weight [g/mol]:	128.17
CAS:	2210-28-8

Physical Properties

Property code	Value	Unit	Source
gf	-146.57	kJ/mol	Joback Method
hf	-316.97	kJ/mol	Joback Method
hfus	14.08	kJ/mol	Joback Method
hvap	39.74	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	856.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	856.00		NIST Webbook
ripol	1137.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1137.00		NIST Webbook
tb	432.41	K	Joback Method
tc	615.89	K	Joback Method
tf	225.09	K	Joback Method

vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.80	J/mol×K	432.41	Joback Method
cpg	233.44	J/mol×K	462.99	Joback Method
cpg	243.68	J/mol×K	493.57	Joback Method
cpg	253.52	J/mol×K	524.15	Joback Method
cpg	262.97	J/mol×K	554.73	Joback Method
cpg	272.04	J/mol×K	585.31	Joback Method
cpg	280.72	J/mol×K	615.89	Joback Method
hvapt	41.60	kJ/mol	358.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47897e+01
Coeff. B	-3.70758e+03
Coeff. C	-5.62420e+01
Temperature range (K), min.	311.90
Temperature range (K), max.	447.41

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.80078e+01
Coeff. B	-7.86510e+03
Coeff. C	-9.16194e+00
Coeff. D	4.66624e-06
Temperature range (K), min.	223.00
Temperature range (K), max.	599.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1180.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2210288&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1180
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
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