2-Propenoic acid, 1-methylpropyl ester

Other names:	Acrylic acid, sec-butyl ester
	s-Butyl acrylate
	sec-Butyl Acrylate
Inchi:	InChI=1S/C7H12O2/c1-4-6(3)9-7(8)5-2/h5-6H,2,4H2,1,3H3
InchiKey:	RNOOHTVUSNIPCJ-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	C=CC(=O)OC(C)CC
Mol. weight [g/mol]:	128.17
CAS:	2998-08-5

Physical Properties

Property code	Value	Unit	Source
gf	-140.46	kJ/mol	Joback Method
hf	-312.46	kJ/mol	Joback Method
hfus	11.87	kJ/mol	Joback Method
hvap	39.27	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.514		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
tb	432.09	K	Joback Method
tc	616.21	K	Joback Method
tf	224.05	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.93	J/mol×K	432.09	Joback Method
cpg	233.73	J/mol×K	462.78	Joback Method
cpg	244.12	J/mol×K	493.46	Joback Method
cpg	254.10	J/mol×K	524.15	Joback Method
cpg	263.67	J/mol×K	554.84	Joback Method
cpg	272.85	J/mol×K	585.52	Joback Method

cpg	281.64	J/mol×K	616.21	Joback Method
dvisc	0.0042260	Pa×s	224.05	Joback Method
dvisc	0.0019297	Pa×s	258.72	Joback Method
dvisc	0.0010605	Pa×s	293.40	Joback Method
dvisc	0.0006615	Pa×s	328.07	Joback Method
dvisc	0.0004515	Pa×s	362.74	Joback Method
dvisc	0.0003294	Pa×s	397.42	Joback Method
dvisc	0.0002529	Pa×s	432.09	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38311e+01
Coeff. B	-3.38339e+03
Coeff. C	-5.35040e+01
Temperature range (K), min.	303.32
Temperature range (K), max.	450.63

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2998085&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume