2-Butenoic acid, 1-methylethyl ester

Other names:	Crotonic acid, isopropyl ester
	Isopropyl crotonate
	Isopropyl 2-butenoate
	(E)-2-Butenoic acid isopropyl ester
	CH3CH=CHC(O)OCH(CH3)2
	Crotonic acid, isopropyl ester, trans
Inchi:	InChI=1S/C7H12O2/c1-4-5-7(8)9-6(2)3/h4-6H,1-3H3/b5-4+
InchiKey:	AABBHSMFGKYLKE-SNAWJCMRSA-N
Formula:	C7H12O2
SMILES:	CC=CC(=O)OC(C)C
Mol. weight [g/mol]:	128.17
CAS:	18060-77-0

Physical Properties

Property code	Value	Unit	Source
chl	-4012.50 ± 2.50	kJ/mol	NIST Webbook
gf	-148.08	kJ/mol	Joback Method
hf	-411.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-457.00 ± 3.00	kJ/mol	NIST Webbook
hfus	13.35	kJ/mol	Joback Method
hvap	46.00	kJ/mol	NIST Webbook
hvap	46.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-1.58		Crippen Method
logp	1.514		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	863.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	864.00		NIST Webbook
tb	439.57	K	Joback Method
tc	628.84	K	Joback Method
tf	220.73	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.78	J/mol×K	439.57	Joback Method
cpg	233.88	J/mol×K	471.11	Joback Method
cpg	244.50	J/mol×K	502.66	Joback Method
cpg	254.66	J/mol×K	534.20	Joback Method
cpg	264.37	J/mol×K	565.75	Joback Method
cpg	273.65	J/mol×K	597.29	Joback Method
cpg	282.49	J/mol×K	628.84	Joback Method
dvisc	0.0044540	Pa×s	220.73	Joback Method
dvisc	0.0018688	Pa×s	257.20	Joback Method
dvisc	0.0009729	Pa×s	293.68	Joback Method
dvisc	0.0005850	Pa×s	330.15	Joback Method
dvisc	0.0003893	Pa×s	366.62	Joback Method
dvisc	0.0002788	Pa×s	403.10	Joback Method
dvisc	0.0002111	Pa×s	439.57	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18060770&Units=SI
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

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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