Propanoic acid, 1-methylpropyl ester

Other names:	1-Methylpropyl propanoate
	Propionic acid, sec-butyl ester
	sec-Butyl propionate
Inchi:	InChI=1S/C7H14O2/c1-4-6(3)9-7(8)5-2/h6H,4-5H2,1-3H3
InchiKey:	VPSLGSSVPWVZFG-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCC(=O)OC(C)CC
Mol. weight [g/mol]:	130.18
CAS:	591-34-4

Physical Properties

Property code	Value	Unit	Source
chl	-4185.30	kJ/mol	NIST Webbook
gf	-228.30	kJ/mol	Joback Method
hf	-437.89	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	39.94	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.738		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	847.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	845.00		NIST Webbook
ripol	1065.00		NIST Webbook
ripol	1092.00		NIST Webbook
ripol	1048.00		NIST Webbook
ripol	1070.00		NIST Webbook
ripol	1067.00		NIST Webbook
tb	406.20	K	NIST Webbook
tc	615.76	K	Joback Method
tf	225.81	K	Joback Method

vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.73	J/mol×K	435.41	Joback Method
cpg	250.17	J/mol×K	465.47	Joback Method
cpg	261.22	J/mol×K	495.53	Joback Method
cpg	271.87	J/mol×K	525.58	Joback Method
cpg	282.12	J/mol×K	555.64	Joback Method
cpg	291.98	J/mol×K	585.70	Joback Method
cpg	301.45	J/mol×K	615.76	Joback Method
dvisc	0.0047724	Pa×s	225.81	Joback Method
dvisc	0.0021099	Pa×s	260.74	Joback Method
dvisc	0.0011312	Pa×s	295.68	Joback Method
dvisc	0.0006919	Pa×s	330.61	Joback Method
dvisc	0.0004649	Pa×s	365.54	Joback Method
dvisc	0.0003348	Pa×s	400.48	Joback Method
dvisc	0.0002542	Pa×s	435.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50392e+01
Coeff. B	-3.66963e+03
Coeff. C	-5.40600e+01
Temperature range (K), min.	302.82
Temperature range (K), max.	431.29

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C591344&Units=SI

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

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

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
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
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