Propanoic acid, 1-methylethyl ester

Other names:	1-methylethyl propanoate
	2-propyl propanoate
	C2H5C(O)OCH(CH3)2
	Isopropyl ester of propanoic acid
	Propionic acid, isopropyl ester
	UN 2409
	iso-Propyl n-propionate
	iso-Propyl propanoate
	isopropyl propanoate
	isopropyl propionate
Inchi:	InChI=1S/C6H12O2/c1-4-6(7)8-5(2)3/h5H,4H2,1-3H3
InchiKey:	IJMWOMHMDSDKGK-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCC(=O)OC(C)C
Mol. weight [g/mol]:	116.16
CAS:	637-78-5

Physical Properties

Property code	Value	Unit	Source
chl	-3531.00	kJ/mol	NIST Webbook
gf	-236.72	kJ/mol	Joback Method
hf	-417.25	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	37.72	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.348		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	740.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	742.00		NIST Webbook

rinpol	717.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	751.00		NIST Webbook
ripol	970.00		NIST Webbook
ripol	950.00		NIST Webbook
ripol	986.00		NIST Webbook
ripol	996.00		NIST Webbook
ripol	956.00		NIST Webbook
ripol	948.00		NIST Webbook
ripol	957.00		NIST Webbook
tb	383.15 ± 1.00	K	NIST Webbook
tb	382.65	K	Multiphase equilibria for mixtures containing water, isopropanol, propionic acid, and isopropyl propionate
tc	594.22	K	Joback Method
tf	214.54	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.90	J/mol×K	412.53	Joback Method
cpg	210.06	J/mol×K	442.81	Joback Method
cpg	219.89	J/mol×K	473.09	Joback Method
cpg	229.39	J/mol×K	503.38	Joback Method
cpg	238.55	J/mol×K	533.66	Joback Method
cpg	247.38	J/mol×K	563.94	Joback Method
cpg	255.87	J/mol×K	594.22	Joback Method
dvisc	0.0002624	Pa×s	412.53	Joback Method
dvisc	0.0020807	Pa×s	247.54	Joback Method
dvisc	0.0011317	Pa×s	280.54	Joback Method

dvisc	0.0046134	Pa×s	214.54	Joback Method
dvisc	0.0004742	Pa×s	346.53	Joback Method
dvisc	0.0003438	Pa×s	379.53	Joback Method
dvisc	0.0006998	Pa×s	313.53	Joback Method
pvap	24.60	kPa	337.66	Multiphase equilibria for mixtures containing water, isopropanol, propionic acid, and isopropyl propionate
pvap	29.50	kPa	342.61	Multiphase equilibria for mixtures containing water, isopropanol, propionic acid, and isopropyl propionate
pvap	35.68	kPa	347.62	Multiphase equilibria for mixtures containing water, isopropanol, propionic acid, and isopropyl propionate
pvap	42.43	kPa	352.67	Multiphase equilibria for mixtures containing water, isopropanol, propionic acid, and isopropyl propionate
pvap	50.12	kPa	357.58	Multiphase equilibria for mixtures containing water, isopropanol, propionic acid, and isopropyl propionate
pvap	59.00	kPa	362.57	Multiphase equilibria for mixtures containing water, isopropanol, propionic acid, and isopropyl propionate
pvap	101.30	kPa	382.65	Multiphase equilibria for mixtures containing water, isopropanol, propionic acid, and isopropyl propionate

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C637785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Multiphase equilibria for mixtures containing water, isopropanol, propionic acid, and isopropyl propionate:	https://www.doi.org/10.1016/j.fluid.2011.03.003
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