Propanoic acid, 2-methyl-, ethyl ester

Other names:	2-Methylpropanoic acid ethyl ester
	ETHYL 2-METHYLPROPANOATE
	ETHYL ESTER ISOBUTYRIC ACID
	Ethyl 2,2-dimethylacetate
	Ethyl 2-methylpropionate
	Ethyl ester of 2-methyl-propanoic acid
	Ethyl isobutanoate
	Ethyl isobutyrate
	Ethyl methylpropanoate
	Ethyl-2-methylproanoate
	Isobutyric acid, ethyl ester
	NSC 97194
	Propionic acid, 2-methyl-, ethyl ester
	UN 2385
Inchi:	InChI=1S/C6H12O2/c1-4-8-6(7)5(2)3/h5H,4H2,1-3H3
InchiKey:	WDAXFOBOLVPGLV-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCOC(=O)C(C)C
Mol. weight [g/mol]:	116.16
CAS:	97-62-1

Physical Properties

Property code	Value	Unit	Source
af	0.4310		KDB
dm	2.10	debye	KDB
gf	-236.72	kJ/mol	Joback Method
hf	-417.25	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	39.80 ± 0.10	kJ/mol	NIST Webbook
hvap	35.60 ± 0.04	kJ/mol	NIST Webbook
hvap	39.88	kJ/mol	NIST Webbook
hvap	39.80 ± 0.10	kJ/mol	NIST Webbook
log10ws	-0.95		Crippen Method
logp	1.205		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3053.00 ± 202.65	kPa	NIST Webbook
pc	3070.00	kPa	KDB

rhoc	276.46 ± 8.13	kg/m3	NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	750.00		NIST Webbook
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rinpol	756.00		NIST Webbook
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rinpol	726.00		NIST Webbook
rinpol	755.70		NIST Webbook
rinpol	743.00		NIST Webbook
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ripol	961.00		NIST Webbook
ripol	950.00		NIST Webbook
ripol	968.00		NIST Webbook
tb	383.20	K	KDB
tc	553.00	K	KDB
tc	553.60 ± 4.00	K	NIST Webbook

tf	184.90	K	KDB
tf	175.40 ± 0.30	K	NIST Webbook
vc	0.421	m3/kmol	KDB
zc	0.2810990		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.90	J/mol×K	412.53	Joback Method
cpg	219.89	J/mol×K	473.09	Joback Method
cpg	255.87	J/mol×K	594.22	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	210.06	J/mol×K	442.81	Joback Method
dvisc	0.0003438	Pa×s	379.53	Joback Method
dvisc	0.0004742	Pa×s	346.53	Joback Method
dvisc	0.0006998	Pa×s	313.53	Joback Method
dvisc	0.0011317	Pa×s	280.54	Joback Method
dvisc	0.0020807	Pa×s	247.54	Joback Method
dvisc	0.0002624	Pa×s	412.53	Joback Method
dvisc	0.0046134	Pa×s	214.54	Joback Method
hvapt	44.10	kJ/mol	321.00	NIST Webbook
hvapt	36.00	kJ/mol	433.00	NIST Webbook
hvapt	33.67	kJ/mol	383.30	NIST Webbook
rhol	836.05	kg/m3	323.15	Vapor-liquid equilibrium and excess properties of the binary mixtures formed by ethyl isobutyrate and n-alkanols
rhol	857.92	kg/m3	303.15	Vapor-liquid equilibrium and excess properties of the binary mixtures formed by ethyl isobutyrate and n-alkanols
rhol	869.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48292e+01
Coeff. B	-3.42855e+03
Coeff. C	-4.76240e+01
Temperature range (K), min.	283.40
Temperature range (K), max.	407.85

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.61664e+01
Coeff. B	-5.99692e+03
Coeff. C	-4.38282e+00
Coeff. D	1.12312e-06
Temperature range (K), min.	185.00
Temperature range (K), max.	553.15

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97621&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor-liquid equilibrium and excess properties of the binary mixtures formed by ethyl isobutyrate and n-alkanols:	https://www.doi.org/10.1016/j.jct.2019.105884
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1077
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1077.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
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
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
rhoc:	Critical density
rhol:	Liquid Density
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
zc:	Critical Compressibility

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