

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	39.88	kJ/mol	NIST Webbook
hvap	35.60 ± 0.04	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	3070.00	kPa	KDB
pc	3053.00 ± 202.65	kPa	NIST Webbook

rhoc	276.46 ± 8.13	kg/m3	NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	755.70		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	754.00		NIST Webbook
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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	238.55	J/mol×K	533.66	Joback Method
cpg	255.87	J/mol×K	594.22	Joback Method
cpg	247.38	J/mol×K	563.94	Joback Method
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
dvisc	0.0004742	Pa×s	346.53	Joback Method
dvisc	0.0003438	Pa×s	379.53	Joback Method
dvisc	0.0002624	Pa×s	412.53	Joback Method
dvisc	0.0046134	Pa×s	214.54	Joback Method
dvisc	0.0020807	Pa×s	247.54	Joback Method
dvisc	0.0011317	Pa×s	280.54	Joback Method
dvisc	0.0006998	Pa×s	313.53	Joback Method
hvapt	44.10	kJ/mol	321.00	NIST Webbook
hvapt	33.67	kJ/mol	383.30	NIST Webbook
hvapt	36.00	kJ/mol	433.00	NIST Webbook
rho1	836.05	kg/m3	323.15	Vapor-liquid equilibrium and excess properties of the binary mixtures formed by ethyl isobutyrate and n-alkanols
rho1	857.92	kg/m3	303.15	Vapor-liquid equilibrium and excess properties of the binary mixtures formed by ethyl isobutyrate and n-alkanols
rho1	869.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1077
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1077.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97621&Units=SI

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
rho:	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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