

# Formic acid, 2-methylpropyl ester

<b>Other names:</b>	2-Methyl-1-propyl formate 2-Methylpropyl formate 2-methylpropyl methanoate Formic acid, isobutyl ester Isobutyl formate Isobutyl methanoate Isobutylester kyseliny mravenci NSC 6968 Tetryl formate UN 2393 methanoic acid, 2-methylpropyl ester
<b>Inchi:</b>	InChI=1S/C5H10O2/c1-5(2)3-7-4-6/h4-5H,3H2,1-2H3
<b>InchiKey:</b>	AVMSWPWPYJVYKY-UHFFFAOYSA-N
<b>Formula:</b>	C5H10O2
<b>SMILES:</b>	CC(C)COC=O
<b>Mol. weight [g/mol]:</b>	102.13
<b>CAS:</b>	542-55-2

## Physical Properties

Property code	Value	Unit	Source
af	0.3960		KDB
dm	1.90	debye	KDB
gf	-215.74	kJ/mol	Joback Method
hf	-369.61	kJ/mol	Joback Method
hfus	8.66	kJ/mol	Joback Method
hvap	33.60 ± 0.04	kJ/mol	NIST Webbook
ie	10.46 ± 0.02	eV	NIST Webbook
log10ws	-1.01		Estimated Solubility Method
log10ws	-1.01		Aqueous Solubility Prediction Method
logp	0.815		Crippen Method
mvol	88.750	ml/mol	McGowan Method
pc	3880.00	kPa	KDB
pc	3880.00 ± 303.98	kPa	NIST Webbook
rhoc	287.91 ± 5.11	kg/m3	NIST Webbook
rinpol	670.00		NIST Webbook

rinpol	670.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	670.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	670.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	642.00		NIST Webbook
ripol	955.00		NIST Webbook
ripol	955.00		NIST Webbook
tb	371.55 ± 0.50	K	NIST Webbook
tb	370.00 ± 3.00	K	NIST Webbook
tb	370.90 ± 0.50	K	NIST Webbook
tb	369.75 ± 1.00	K	NIST Webbook
tb	371.25 ± 1.00	K	NIST Webbook
tb	371.05 ± 1.00	K	NIST Webbook
tb	371.60 ± 0.40	K	NIST Webbook
tb	371.40	K	KDB
tb	371.60	K	NIST Webbook
tb	371.45 ± 0.30	K	NIST Webbook
tb	370.40 ± 1.00	K	NIST Webbook
tb	371.10 ± 0.50	K	NIST Webbook
tb	371.10 ± 0.50	K	NIST Webbook
tb	371.65 ± 1.00	K	NIST Webbook
tc	551.00	K	KDB
tc	551.40 ± 4.00	K	NIST Webbook
tf	177.35	K	Aqueous Solubility Prediction Method
tf	177.90 ± 0.40	K	NIST Webbook
tf	177.30	K	KDB
vc	0.352	m <sup>3</sup> /kmol	KDB
zc	0.2981170		KDB

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.22	J/mol×K	532.38	Joback Method
cpg	197.81	J/mol×K	502.79	Joback Method
cpg	190.13	J/mol×K	473.21	Joback Method
cpg	182.20	J/mol×K	443.62	Joback Method

cpg	174.02	J/molxK	414.03	Joback Method
cpg	165.58	J/molxK	384.44	Joback Method
cpg	212.38	J/molxK	561.97	Joback Method
cpl	214.20	J/molxK	290.00	NIST Webbook
dvisc	0.0048899	Paxs	195.34	Joback Method
dvisc	0.0002815	Paxs	384.44	Joback Method
dvisc	0.0003663	Paxs	352.92	Joback Method
dvisc	0.0005019	Paxs	321.41	Joback Method
dvisc	0.0007365	Paxs	289.89	Joback Method
dvisc	0.0011867	Paxs	258.37	Joback Method
dvisc	0.0021832	Paxs	226.86	Joback Method
hvapt	38.60	kJ/mol	306.00	NIST Webbook
hvapt	36.60	kJ/mol	439.00	NIST Webbook
rho1	885.00	kg/m3	293.00	KDB

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45847e+01
Coeff. B	-3.09930e+03
Coeff. C	-6.00250e+01
Temperature range (K), min.	276.80
Temperature range (K), max.	394.24

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	-1.77684e+01
Coeff. B	-3.64340e+03
Coeff. C	5.72239e+00
Coeff. D	-1.18607e-05
Temperature range (K), min.	177.35
Temperature range (K), max.	551.35

# Sources

<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>KDB:</b>	<a href="https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1069">https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1069</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>KDB Vapor Pressure Data:</b>	<a href="https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1069">https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1069</a>
<b>Assessment, measurement and correlation of (vapour + liquid) equilibria in (carbon dioxide + butyl, isobutyl and amyl formate) systems: Estimated Solubility Method:</b>	<a href="https://www.doi.org/10.1016/j.jct.2013.05.017">https://www.doi.org/10.1016/j.jct.2013.05.017</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C542552&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C542552&amp;Units=SI</a>

# Legend

<b>af:</b>	Acentric Factor
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>dm:</b>	Dipole Moment
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rhoc:</b>	Critical density
<b>rhoL:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

**zc:** Critical Compressibility

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