Formic acid, 1-methylethyl ester

Other names:	Formic acid, 2-propyl ester
	Formic acid, isopropyl ester
	HCOOCH(CH3)2
	Isopropyl formate
	Methylethyl formate
	UN 1281
Inchi:	InChI=1S/C4H8O2/c1-4(2)6-3-5/h3-4H,1-2H3
InchiKey:	RMOUBSOVHSONPZ-UHFFFAOYSA-N
Formula:	C4H8O2
SMILES:	CC(C)OC=O
Mol. weight [g/mol]:	88.11
CAS:	625-55-8

Physical Properties

Property code	Value	Unit	Source
affp	811.30	kJ/mol	NIST Webbook
basg	780.30	kJ/mol	NIST Webbook
gf	-224.16	kJ/mol	Joback Method
hf	-348.97	kJ/mol	Joback Method
hfus	6.07	kJ/mol	Joback Method
hvap	33.24	kJ/mol	Joback Method
ie	10.44	eV	NIST Webbook
ie	10.44 ± 0.05	eV	NIST Webbook
log10ws	-0.63		Aqueous Solubility Prediction Method
log10ws	-0.63		Estimated Solubility Method
logp	0.568		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
rinpol	529.00		NIST Webbook
rinpol	532.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	525.00		NIST Webbook
rinpol	573.00		NIST Webbook
rinpol	562.00		NIST Webbook
rinpol	559.00		NIST Webbook

rinpol	559.00		NIST Webbook
rinpol	528.00		NIST Webbook
rinpol	567.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	516.00		NIST Webbook
rinpol	516.00		NIST Webbook
rinpol	567.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	532.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	552.00		NIST Webbook
ripol	883.00		NIST Webbook
ripol	838.00		NIST Webbook
ripol	851.00		NIST Webbook
ripol	838.00		NIST Webbook
ripol	840.00		NIST Webbook
ripol	838.00		NIST Webbook
tb	342.00 ± 0.40	K	NIST Webbook
tb	341.40	K	NIST Webbook
tc	539.67	K	Joback Method
tf	186.65	K	Aqueous Solubility Prediction Method
vc	0.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.62	J/mol×K	539.67	Joback Method
cpg	131.99	J/mol×K	361.56	Joback Method
cpg	138.90	J/mol×K	391.25	Joback Method
cpg	145.62	J/mol×K	420.93	Joback Method
cpg	152.16	J/mol×K	450.62	Joback Method
cpg	158.51	J/mol×K	480.30	Joback Method
cpg	164.66	J/mol×K	509.99	Joback Method
dvisc	0.0002752	Pa×s	361.56	Joback Method
dvisc	0.0044029	Pa×s	184.07	Joback Method
dvisc	0.0020143	Pa×s	213.65	Joback Method
dvisc	0.0011146	Pa×s	243.23	Joback Method
dvisc	0.0007012	Pa×s	272.81	Joback Method
dvisc	0.0004830	Pa×s	302.40	Joback Method

dvisc	0.0003555	Pa×s	331.98	Joback Method
hvapt	34.50	kJ/mol	281.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37050e+01
Coeff. B	-2.40986e+03
Coeff. C	-7.61910e+01
Temperature range (K), min.	255.80
Temperature range (K), max.	363.30

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C625558&Units=SI

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

Legend

affp: Proton affinity

basg: Gas basicity

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

hvapt: Enthalpy of vaporization at a given temperature

ie:	Ionization energy
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