Formic acid, 1-methylpropyl ester

Other names:	Formic acid, sec-butyl ester
	butan-2-yl formate
	s-Butyl formate
	sec-Butyl Formate
	sec-Butyl methanoate
Inchi:	InChI=1S/C5H10O2/c1-3-5(2)7-4-6/h4-5H,3H2,1-2H3
InchiKey:	OAEQYDZVVPONKW-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CCC(C)OC=O
Mol. weight [g/mol]:	102.13
CAS:	589-40-2

Physical Properties

Property code	Value	Unit	Source
gf	-215.74	kJ/mol	Joback Method
hf	-369.61	kJ/mol	Joback Method
hfus	8.66	kJ/mol	Joback Method
hvap	35.47	kJ/mol	Joback Method
log10ws	-0.89		Crippen Method
logp	0.958		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
rinpol	633.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	633.00		NIST Webbook
tb	384.44	K	Joback Method
tc	561.97	K	Joback Method
tf	195.34	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.58	J/mol×K	384.44	Joback Method
cpg	174.02	J/mol×K	414.03	Joback Method
cpg	182.20	J/mol×K	443.62	Joback Method
cpg	190.13	J/mol×K	473.21	Joback Method
cpg	197.81	J/mol×K	502.79	Joback Method
cpg	205.22	J/mol×K	532.38	Joback Method
cpg	212.38	J/mol×K	561.97	Joback Method
dvisc	0.0048899	Pa×s	195.34	Joback Method
dvisc	0.0021832	Pa×s	226.86	Joback Method
dvisc	0.0011867	Pa×s	258.37	Joback Method
dvisc	0.0007365	Pa×s	289.89	Joback Method
dvisc	0.0005019	Pa×s	321.41	Joback Method
dvisc	0.0003663	Pa×s	352.92	Joback Method
dvisc	0.0002815	Pa×s	384.44	Joback Method
hvapt	37.70	kJ/mol	302.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29998e+01
Coeff. B	-2.47209e+03
Coeff. C	-7.80530e+01
Temperature range (K), min.	272.52
Temperature range (K), max.	399.59

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C589402&Units=SI

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

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

Legend

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume