Formic acid, 1,1-dimethylethyl ester

Other names:	Formic acid, tert-butyl ester
	tert-Butyl Formate
Inchi:	InChI=1S/C5H10O2/c1-5(2,3)7-4-6/h4H,1-3H3
InchiKey:	RUPAXCPQAAOIPB-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CC(C)(C)OC=O
Mol. weight [g/mol]:	102.13
CAS:	762-75-4

Physical Properties

Property code	Value	Unit	Source
gf	-210.46	kJ/mol	Joback Method
hf	-456.80 ± 5.40	kJ/mol	NIST Webbook
hfl	-493.00 ± 3.00	kJ/mol	NIST Webbook
hfus	4.77	kJ/mol	Joback Method
hvap	36.20	kJ/mol	NIST Webbook
hvap	36.30 ± 4.20	kJ/mol	NIST Webbook
log10ws	-0.89		Crippen Method
logp	0.958		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	585.00		NIST Webbook
rinpol	589.00		NIST Webbook
rinpol	589.00		NIST Webbook
tb	355.70	K	NIST Webbook
tb	356.15 ± 1.00	K	NIST Webbook
tb	356.00 ± 1.50	K	NIST Webbook
tc	566.82	K	Joback Method
tf	212.76	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	167.22	J/mol×K	381.65	Joback Method
cpg	210.30	J/mol×K	535.96	Joback Method
cpg	202.49	J/mol×K	505.10	Joback Method
cpg	194.29	J/mol×K	474.24	Joback Method
cpg	185.68	J/mol×K	443.37	Joback Method
cpg	176.66	J/mol×K	412.51	Joback Method
cpg	217.73	J/mol×K	566.82	Joback Method
dvisc	0.0003279	Pa×s	381.65	Joback Method
dvisc	0.0004333	Pa×s	353.50	Joback Method
dvisc	0.0006010	Pa×s	325.35	Joback Method
dvisc	0.0008869	Pa×s	297.20	Joback Method
dvisc	0.0014196	Pa×s	269.06	Joback Method
dvisc	0.0025365	Pa×s	240.91	Joback Method
dvisc	0.0052844	Pa×s	212.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35549e+01
Coeff. B	-2.43235e+03
Coeff. C	-8.35210e+01
Temperature range (K), min.	266.86
Temperature range (K), max.	378.59

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C762754&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

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

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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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