Nitric acid, 1-methylethyl ester

Other names:	(CH3)2CHONO2
	Isopropyl nitrate
	Isopropylester kyseliny dusicne
	Nitric acid, isopropyl ester
	UN 1222
Inchi:	InChI=1S/C3H7NO3/c1-3(2)7-4(5)6/h3H,1-2H3
InchiKey:	GAPFWGOSHOCNBM-UHFFFAOYSA-N
Formula:	C3H7NO3
SMILES:	CC(C)O[N+](=O)[O-]
Mol. weight [g/mol]:	105.09
CAS:	1712-64-7

Physical Properties

Property code	Value	Unit	Source
chl	-1954.90 ± 2.00	kJ/mol	NIST Webbook
chl	-1951.00 ± 1.00	kJ/mol	NIST Webbook
gf	-97.51	kJ/mol	Joback Method
hf	-253.51	kJ/mol	Joback Method
hfl	-226.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-230.00 ± 1.00	kJ/mol	NIST Webbook
hfus	12.55	kJ/mol	Joback Method
hvap	38.79	kJ/mol	NIST Webbook
log10ws	-1.35		Crippen Method
logp	0.603		Crippen Method
mcvol	76.420	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
rinpol	684.30		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	663.80		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	663.80		NIST Webbook
rinpol	664.00		NIST Webbook
sl	263.20	J/mol×K	NIST Webbook
tb	373.70	K	NIST Webbook
tc	655.21	K	Joback Method
tf	274.41	K	Joback Method

tt	190.81 ± 0.02	K	NIST Webbook
vc	0.297	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.26	J/mol×K	441.86	Joback Method
cpg	189.66	J/mol×K	619.65	Joback Method
cpg	183.03	J/mol×K	584.10	Joback Method
cpg	176.07	J/mol×K	548.54	Joback Method
cpg	168.78	J/mol×K	512.98	Joback Method
cpg	161.18	J/mol×K	477.42	Joback Method
cpg	195.96	J/mol×K	655.21	Joback Method
cpl	200.70	J/mol×K	350.00	NIST Webbook
cpl	191.10	J/mol×K	298.15	NIST Webbook
hfust	10.10	kJ/mol	190.90	NIST Webbook
hfust	10.10	kJ/mol	190.90	NIST Webbook
hfust	10.01	kJ/mol	190.81	NIST Webbook
hvapt	39.70	kJ/mol	308.00	NIST Webbook
sfust	52.43	J/mol×K	190.81	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48459e+01
Coeff. B	-3.36152e+03
Coeff. C	-4.50270e+01
Temperature range (K), min.	275.93
Temperature range (K), max.	397.59

Sources

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=C1712647&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume