Nitric acid, propyl ester

Other names:	Monopropyl nitrate
	Nitrate de propyle normal
	Propyl nitrate
	Propylester kyseliny dusicne
	UN 1865
	n-C3H7ONO2
	n-Propyl nitrate
Inchi:	InChI=1S/C3H7NO3/c1-2-3-7-4(5)6/h2-3H2,1H3
InchiKey:	JNTOKFNBDFMTIV-UHFFFAOYSA-N
Formula:	C3H7NO3
SMILES:	CCCO[N+](=O)[O-]
Mol. weight [g/mol]:	105.09
CAS:	627-13-4

Physical Properties

Property code	Value	Unit	Source
chl	-1966.00 ± 1.00	kJ/mol	NIST Webbook
gf	-95.07	kJ/mol	Joback Method
hf	-248.23	kJ/mol	Joback Method
hfl	-215.00 ± 1.00	kJ/mol	NIST Webbook
hfus	16.07	kJ/mol	Joback Method
hvap	40.58	kJ/mol	NIST Webbook
ie	11.07 ± 0.02	eV	NIST Webbook
log10ws	-1.24		Crippen Method
logp	0.605		Crippen Method
mcvol	76.420	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
rinpol	700.00		NIST Webbook
rinpol	700.00		NIST Webbook
tb	383.70 ± 0.50	K	NIST Webbook
tb	383.60 ± 1.50	K	NIST Webbook
tc	650.60	K	Joback Method
tf	289.41	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.09	J/mol×K	442.30	Joback Method
cpg	160.73	J/mol×K	477.02	Joback Method
cpg	168.08	J/mol×K	511.73	Joback Method
cpg	175.13	J/mol×K	546.45	Joback Method
cpg	181.89	J/mol×K	581.17	Joback Method
cpg	188.34	J/mol×K	615.88	Joback Method
cpg	194.49	J/mol×K	650.60	Joback Method
hvapt	41.70	kJ/mol	308.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48152e+01
Coeff. B	-3.42648e+03
Coeff. C	-4.76680e+01
Temperature range (K), min.	283.53
Temperature range (K), max.	408.21

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C627134&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume