Nitric acid, ethyl ester

Other names:	C2H5ONO2
	Ethyl nitrate
	Ethylester kyseliny dusicne
	NA 1993
	Nitric ether
Inchi:	InChI=1S/C2H5NO3/c1-2-6-3(4)5/h2H2,1H3
InchiKey:	IDNUEBSJWINEMI-UHFFFAOYSA-N
Formula:	C2H5NO3
SMILES:	CCO[N+](=O)[O-]
Mol. weight [g/mol]:	91.07
CAS:	625-58-1

Physical Properties

Property code	Value	Unit	Source
chl	-1311.20 ± 0.96	kJ/mol	NIST Webbook
gf	-103.49	kJ/mol	Joback Method
hf	-155.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-190.40 ± 1.00	kJ/mol	NIST Webbook
hfl	-191.00 ± 3.00	kJ/mol	NIST Webbook
hfus	13.48	kJ/mol	Joback Method
hvap	36.28	kJ/mol	NIST Webbook
hvap	36.00	kJ/mol	NIST Webbook
ie	11.22	eV	NIST Webbook
log10ws	-0.82		Crippen Method
logp	0.215		Crippen Method
mcvol	62.330	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
rinpol	631.50		NIST Webbook
rinpol	611.90		NIST Webbook
ripol	969.00		NIST Webbook
ripol	969.00		NIST Webbook
sl	247.20	J/mol×K	NIST Webbook
tb	360.90 ± 0.50	K	NIST Webbook
tb	361.90 ± 0.50	K	NIST Webbook
tb	361.85 ± 0.30	K	NIST Webbook
tb	360.75 ± 1.50	K	NIST Webbook
tb	360.40	K	NIST Webbook

tc	630.25	K	Joback Method
tf	171.15 ± 0.60	K	NIST Webbook
tt	178.60 ± 0.20	K	NIST Webbook
vc	0.247	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.58	J/mol×K	630.25	Joback Method
cpg	145.65	J/mol×K	595.11	Joback Method
cpg	140.48	J/mol×K	559.97	Joback Method
cpg	135.09	J/mol×K	524.83	Joback Method
cpg	129.49	J/mol×K	489.70	Joback Method
cpg	123.67	J/mol×K	454.56	Joback Method
cpg	117.65	J/mol×K	419.42	Joback Method
cpl	170.30	J/mol×K	298.00	NIST Webbook
hfust	8.53	kJ/mol	178.60	NIST Webbook
hfust	8.53	kJ/mol	178.60	NIST Webbook
hfust	8.53	kJ/mol	178.60	NIST Webbook
hvapt	37.00	kJ/mol	303.00	NIST Webbook
hvapt	37.30	kJ/mol	308.00	NIST Webbook
hvapt	37.00	kJ/mol	317.00	NIST Webbook
sfust	47.74	J/mol×K	178.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48158e+01
Coeff. B	-3.25371e+03
Coeff. C	-4.13300e+01
Temperature range (K), min.	265.29
Temperature range (K), max.	383.67

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=C625581&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
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
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

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