Methyl nitrate

Other names:	CH3ONO2
	METHYL ESTER
	Methylester kyseliny dusicne
	NITRIC ACID
	Nitric acid, methyl ester
Inchi:	InChI=1S/CH3NO3/c1-5-2(3)4/h1H3
InchiKey:	LRMHVVPPGGOAJQ-UHFFFAOYSA-N
Formula:	CH3NO3
SMILES:	CO[N+](=O)[O-]
Mol. weight [g/mol]:	77.04
CAS:	598-58-3

Physical Properties

Property code	Value	Unit	Source
affp	733.60	kJ/mol	NIST Webbook
basg	714.80	kJ/mol	NIST Webbook
gf	-111.91	kJ/mol	Joback Method
hf	-122.00 ± 1.00	kJ/mol	NIST Webbook
hfus	10.89	kJ/mol	Joback Method
hvap	34.10	kJ/mol	NIST Webbook
ie	11.53 ± 0.01	eV	NIST Webbook
log10ws	-0.40		Crippen Method
logp	-0.176		Crippen Method
mcvol	48.240	ml/mol	McGowan Method
pc	5747.92	kPa	Joback Method
rinpol	548.00		NIST Webbook
rinpol	525.00		NIST Webbook
sl	216.98	J/mol×K	NIST Webbook
tb	338.15 ± 1.50	K	NIST Webbook
tb	337.75	K	KDB
tb	338.15 ± 1.50	K	NIST Webbook
tb	338.00 ± 0.50	K	NIST Webbook
tc	609.66	K	Joback Method
tf	190.19	K	KDB
tt	190.20 ± 0.10	K	NIST Webbook
vc	0.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	93.01	J/mol×K	467.58	Joback Method
cpg	108.23	J/mol×K	609.66	Joback Method
cpg	104.64	J/mol×K	574.14	Joback Method
cpg	100.89	J/mol×K	538.62	Joback Method
cpg	97.02	J/mol×K	503.10	Joback Method
cpg	84.67	J/mol×K	396.54	Joback Method
cpg	88.90	J/mol×K	432.06	Joback Method
cpl	157.19	J/mol×K	298.20	NIST Webbook
hfust	8.24	kJ/mol	190.20	NIST Webbook
hfust	8.24	kJ/mol	190.20	NIST Webbook
hfust	8.24	kJ/mol	190.20	NIST Webbook
hvapt	34.80	kJ/mol	288.00	NIST Webbook
sfust	43.33	J/mol×K	190.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49000e+01
Coeff. B	-3.11085e+03
Coeff. C	-3.54360e+01
Temperature range (K), min.	248.33
Temperature range (K), max.	361.42

Sources

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1422

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C598583&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

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
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