Methane, tetranitro-

Other names:	NCI-C55947
	Rcra waste number P112
	TETRANITROMETHANE
	TNM
	UN 1510
Inchi:	InChI=1S/CN4O8/c6-2(7)1(3(8)9,4(10)11)5(12)13
InchiKey:	NYTOUQBROMCLBJ-UHFFFAOYSA-N
Formula:	CN4O8
SMILES:	O=[N+]([O-])C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	196.03
CAS:	509-14-8

Physical Properties

Property code	Value	Unit	Source
chl	-432.00 ± 2.00	kJ/mol	NIST Webbook
chl	-434.70 ± 4.20	kJ/mol	NIST Webbook
gf	102.58	kJ/mol	Joback Method
hf	82.00 ± 2.00	kJ/mol	NIST Webbook
hfl	38.00 ± 2.00	kJ/mol	NIST Webbook
hfl	41.20 ± 4.20	kJ/mol	NIST Webbook
hfl	37.00 ± 3.00	kJ/mol	NIST Webbook
hfus	36.38	kJ/mol	Joback Method
hvap	49.96	kJ/mol	NIST Webbook
hvap	43.90 ± 0.40	kJ/mol	NIST Webbook
ie	12.55	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	-1.296		Crippen Method
mcvol	94.630	ml/mol	McGowan Method
pc	6430.83	kPa	Joback Method
tb	399.20	K	NIST Webbook
tc	1137.98	K	Joback Method
tf	287.05 ± 0.20	K	NIST Webbook
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.80	J/mol×K	826.41	Joback Method
cpg	260.87	J/mol×K	1086.06	Joback Method
cpg	258.80	J/mol×K	1034.13	Joback Method
cpg	256.48	J/mol×K	982.20	Joback Method
cpg	253.80	J/mol×K	930.27	Joback Method
cpg	250.61	J/mol×K	878.34	Joback Method
cpg	262.82	J/mol×K	1137.98	Joback Method
hsubt	47.40	kJ/mol	270.50	NIST Webbook
hvapt	43.10 ± 2.10	kJ/mol	313.00	NIST Webbook
hvapt	40.74	kJ/mol	399.20	NIST Webbook
hvapt	46.60	kJ/mol	293.00	NIST Webbook
hvapt	42.90	kJ/mol	343.00	NIST Webbook
hvapt	43.10	kJ/mol	329.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.71581e+01
Coeff. B	-5.03433e+03
Coeff. C	2.27000e+00
Temperature range (K), min.	291.15
Temperature range (K), max.	422.69

Sources

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1423

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C509148&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

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
hsubt:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume