Tetryl

Other names:	2,4,6-(Trinitrophenyl)methylnitramine 2,4,6-(Trinitrophenyl)methylnitroamine 2,4,6-Tetryl 2,4,6-trinitrophenyl-N-methylnitramine Benzenamine, N-methyl-N,2,4,6-tetranitro- CE N-Methyl-N,2,4,6-tetranitroaniline (tetryl) N-Methyl-N,2,4,6-tetranitrobenzenamine N-Methyl-N-picrylnitramine N-Picryl-N-methylnitramine N-methyl-N,2,4,6-tetranitroaniline N-methyl-N-2,4,6-tetranitrobenzenamine NSC 2166 Nitramine (indicator) Picrylmethylnitramine Picrylnitromethylamine TETRYL (N-methyl-N,2,4,6-tetranitroaniline) Tetralit Tetralite Tetril UN 0208 aniline, N-methyl-N,2,4,6-tetranitro- nitramine
Inchi:	InChI=1S/C7H5N5O8/c1-8(12(19)20)7-5(10(15)16)2-4(9(13)14)3-6(7)11(17)18/h2-3H,1H
InchiKey:	AGUIVNYEYSCPNI-UHFFFAOYSA-N
Formula:	C7H5N5O8
SMILES:	CN(c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	287.14
CAS:	479-45-8

Physical Properties

Property code	Value	Unit	Source
chs	-3495.40 ± 3.50	kJ/mol	NIST Webbook
chs	-3499.86	kJ/mol	NIST Webbook
chs	-3537.00	kJ/mol	NIST Webbook
chs	-3510.00 ± 4.60	kJ/mol	NIST Webbook

chs	-3501.00	kJ/mol	NIST Webbook
chs	-3481.50 ± 2.10	kJ/mol	NIST Webbook
gf	344.56	kJ/mol	Joback Method
hf	38.80	kJ/mol	Joback Method
hfs	41.00 ± 4.60	kJ/mol	NIST Webbook
hfs	30.70	kJ/mol	NIST Webbook
hfus	55.23	kJ/mol	Joback Method
hsub	133.80 ± 1.60	kJ/mol	NIST Webbook
hvap	103.84	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	1.039		Crippen Method
mcvol	165.390	ml/mol	McGowan Method
pc	4119.70	kPa	Joback Method
rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2113.00		NIST Webbook
tb	1020.98	K	Joback Method
tc	1316.45	K	Joback Method
tf	402.60 ± 0.10	K	NIST Webbook
tf	400.50 ± 0.50	K	NIST Webbook
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.30	J/mol×K	1020.98	Joback Method
cpg	483.61	J/mol×K	1070.22	Joback Method
cpg	488.13	J/mol×K	1119.47	Joback Method
cpg	491.93	J/mol×K	1168.71	Joback Method
cpg	495.14	J/mol×K	1217.96	Joback Method
cpg	497.84	J/mol×K	1267.20	Joback Method
cpg	500.15	J/mol×K	1316.45	Joback Method
cps	247.80	J/mol×K	290.00	Thermal conductivity of Tetryl by modulated differential scanning calorimetry

cps	233.16	J/mol×K	270.00	Thermal conductivity of Tetryl by modulated differential scanning calorimetry
cps	278.24	J/mol×K	320.00	Thermal conductivity of Tetryl by modulated differential scanning calorimetry
cps	290.90	J/mol×K	298.00	NIST Webbook
cps	302.10	J/mol×K	298.00	NIST Webbook
cps	260.70	J/mol×K	293.00	NIST Webbook
hfust	25.86	kJ/mol	402.60	NIST Webbook
hfust	22.93	kJ/mol	402.60	NIST Webbook
hfust	25.86	kJ/mol	400.50	NIST Webbook
sfust	57.00	J/mol×K	402.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C479458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal conductivity of Tetryl by modulated differential scanning calorimetry:	https://www.doi.org/10.1016/j.tca.2004.11.033
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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