Trinitrotoluene

Other names:	.alpha.-TNT
	1-Methyl-2,4,6-trinitrobenzene
	2,4,6-TNT
	2,4,6-Trinitrotolueen
	2,4,6-Trinitrotoluene
	2,4,6-Trinitrotoluol
	2-Methyl-1,3,5-Trinitrobenzene
	ALPHA-TNT
	Benzene, 2-methyl-1,3,5-trinitro-
	Gradetol
	NCI-C56155
	NSC 36949
	TNT
	TNT (2,4,6-trinitrotoluene)
	TNT-tolite
	Tolit
	Tolite
	Toluene, 2,4,6-trinitro-
	Tritol
	Tritol (explosive)
	Trojnitrotoluen
	Trotyl
	Trotyl oil
	s-Trinitrotoluene
	s-Trinitrotoluol
	sym-Trinitrotoluene
	sym-Trinitrotoluol
	«alpha»-TNT
	Â«alphaÂ»-TNT
Inchi:	InChI=1S/C7H5N3O6/c1-4-6(9(13)14)2-5(8(11)12)3-7(4)10(15)16/h2-3H,1H3
InchiKey:	SPSSULHKWOKEEL-UHFFFAOYSA-N
Formula:	C7H5N3O6
SMILES:	Cc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	227.13
CAS:	118-96-7

Physical Properties

Property code	Value	Unit	Source
chs	-3419.18	kJ/mol	NIST Webbook
chs	-3388.60 ± 3.00	kJ/mol	NIST Webbook
chs	-3407.00	kJ/mol	NIST Webbook
chs	-3404.50 ± 2.10	kJ/mol	NIST Webbook
chs	-3401.80 ± 3.40	kJ/mol	NIST Webbook
chs	-3402.30 ± 3.40	kJ/mol	NIST Webbook
chs	-3434.00	kJ/mol	NIST Webbook
chs	-3406.00 ± 3.00	kJ/mol	NIST Webbook
gf	198.23	kJ/mol	Joback Method
hf	24.10 ± 3.50	kJ/mol	NIST Webbook
hfs	-49.96	kJ/mol	NIST Webbook
hfs	-80.50 ± 3.10	kJ/mol	NIST Webbook
hfs	-63.20 ± 5.00	kJ/mol	NIST Webbook
hfus	40.84	kJ/mol	Joback Method
hsub	113.20 ± 1.50	kJ/mol	NIST Webbook
hsub	118.00	kJ/mol	NIST Webbook
hsub	104.60 ± 1.70	kJ/mol	NIST Webbook
hsub	105.00 ± 2.00	kJ/mol	NIST Webbook
hvap	87.00 ± 1.90	kJ/mol	NIST Webbook
ie	10.59 ± 0.04	eV	NIST Webbook
log10ws	-3.22		Aqueous Solubility Prediction Method
log10ws	-3.22		Estimated Solubility Method
logp	1.720		Crippen Method
mcvol	137.990	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	1704.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1709.00		NIST Webbook
rinpol	1708.67		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1717.67		NIST Webbook
rinpol	1707.07		NIST Webbook
rinpol	1714.08		NIST Webbook
rinpol	287.66		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1708.67		NIST Webbook
tb	856.70	K	Joback Method
tc	1146.44	K	Joback Method
tf	353.42 ± 0.30	K	NIST Webbook
tf	355.10 ± 0.10	K	NIST Webbook

tf	353.55	K	HP-DSC study of energetic materials. Part I. Overview of pressure influence on thermal behavior
tf	353.20	K	Aqueous Solubility Prediction Method
tf	354.00 ± 2.00	K	NIST Webbook
tf	352.00 ± 0.10	K	NIST Webbook
tf	354.30 ± 0.50	K	NIST Webbook
tt	353.95	K	Thermo-analytical study of a melt cast composition based on cis -1,3,4,6-tetranitrooctahydroimidazo-[4,5 d]imidazole (BCHMX)/trinitrotoluene (TNT) compared with traditional compositions
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.39	J/mol×K	1146.44	Joback Method
cpg	371.64	J/mol×K	856.70	Joback Method
cpg	400.88	J/mol×K	1098.15	Joback Method
cpg	396.66	J/mol×K	1049.86	Joback Method
cpg	391.69	J/mol×K	1001.57	Joback Method
cpg	385.89	J/mol×K	953.28	Joback Method
cpg	379.23	J/mol×K	904.99	Joback Method
cps	311.70	J/mol×K	293.00	NIST Webbook
cps	243.30	J/mol×K	298.00	NIST Webbook
hfust	23.43	kJ/mol	352.20	NIST Webbook
hfust	23.40	kJ/mol	352.20	NIST Webbook
hfust	23.43	kJ/mol	352.20	NIST Webbook
hsubt	99.00 ± 2.00	kJ/mol	313.50	NIST Webbook
hsubt	118.40 ± 4.20	kJ/mol	338.00	NIST Webbook
hsubt	112.40	kJ/mol	323.00	NIST Webbook
hsubt	103.30 ± 2.50	kJ/mol	338.00	NIST Webbook
hvapt	93.70	kJ/mol	438.00	NIST Webbook
hvapt	113.70	kJ/mol	343.15	Comment on Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives

psub	2.71e-04	kPa	338.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.37e-04	kPa	333.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	7.30e-05	kPa	328.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	4.00e-05	kPa	323.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.30e-05	kPa	313.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	2.20e-05	kPa	318.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29612e+01
Coeff. B	-4.32833e+03
Coeff. C	-1.23172e+02
Temperature range (K), min.	464.70
Temperature range (K), max.	688.99

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.87826e+02
Coeff. B	-3.70745e+04
Coeff. C	-8.47236e+01
Coeff. D	5.70032e-05
Temperature range (K), min.	337.15
Temperature range (K), max.	523.15

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C118967&Units=SI

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

Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 293-338 K temperature range: https://www.doi.org/10.1016/j.tca.2010.11.034

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1444

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Comment on Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives: https://www.doi.org/10.1021/acs.jced.6b00483

Thermoanalytical study of a melt cast composition based on cis 1,3,4,6-tetranitrooctahydroimidazo[4,5-d]imidazole (BCHMX)/trinitrotoluene (TNT) compared with traditional compositions: https://www.doi.org/10.1016/j.tca.2018.06.006

HP-DSC study of energetic materials. Part I. Overview of pressure influence on thermal behavior: https://www.doi.org/10.1016/j.tca.2016.03.018

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1444

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume