

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:	<chem>Cc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	227.13
CAS:	118-96-7

Physical Properties

Property code	Value	Unit	Source
chs	-3402.30 ± 3.40	kJ/mol	NIST Webbook
chs	-3406.00 ± 3.00	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	-3419.18	kJ/mol	NIST Webbook
chs	-3434.00	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	22.49	kJ/mol	HP-DSC study of energetic materials. Part I. Overview of pressure influence on thermal behavior
hsub	104.60 ± 1.70	kJ/mol	NIST Webbook
hsub	118.00	kJ/mol	NIST Webbook
hsub	105.00 ± 2.00	kJ/mol	NIST Webbook
hsub	113.20 ± 1.50	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	1717.67		NIST Webbook
rinpol	1708.67		NIST Webbook
rinpol	287.66		NIST Webbook
rinpol	1707.07		NIST Webbook
rinpol	1714.08		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1708.67		NIST Webbook
rinpol	1709.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1704.00		NIST Webbook
tb	856.70	K	Joback Method
tc	1146.44	K	Joback Method
tf	354.00 ± 2.00	K	NIST Webbook

tf	352.00 ± 0.10	K	NIST Webbook
tf	355.10 ± 0.10	K	NIST Webbook
tf	353.42 ± 0.30	K	NIST Webbook
tf	354.30 ± 0.50	K	NIST Webbook
tf	353.20	K	Aqueous Solubility Prediction Method
tf	353.55	K	HP-DSC study of energetic materials. Part I. Overview of pressure influence on thermal behavior
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

hvapt	93.70	kJ/mol	438.00	NIST Webbook
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	2000.00	kPa	353.75	HP-DSC study of energetic materials. Part I. Overview of pressure influence on thermal behavior
psub	1000.00	kPa	353.55	HP-DSC study of energetic materials. Part I. Overview of pressure influence on thermal behavior
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	5000.00	kPa	354.15	HP-DSC study of energetic materials. Part I. Overview of pressure influence on thermal behavior
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	2.20e-05	kPa	318.15	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	10000.00	kPa	354.85	HP-DSC study of energetic materials. Part I. Overview of pressure influence on thermal behavior
psub	14000.00	kPa	355.45	HP-DSC study of energetic materials. Part I. Overview of pressure influence on thermal behavior

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C118967&Units=SI
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
Grimsen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1444
Thermo-analytical study of a melt cast composition based on cis-1,4-bis(4-cyanophenyl)pyridimidazole (BCHMX)/trinitrotoluene (TNT) compared with traditional thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range:	https://www.doi.org/10.1016/j.tca.2018.06.006
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Triacetone triperoxide (TTP) thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range:	https://www.doi.org/10.1016/j.tca.2010.11.034
Estimated Solubility Method:	http://link.springer.com/article/10.1007/BF02311772
Comment on Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives :	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
	https://www.doi.org/10.1021/acs.jced.6b00483

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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