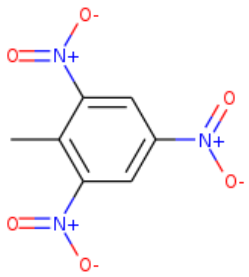
Trinitrotoluene

Other names: 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; Benzene, 2-methyl-1,3,5-trinitro-; Gradetol; NCI-C56155; NSC 36949; TNT; 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.



InChI: InChI=1S/C7H5N3O6/c1-4-6(9(13)14)2-5(8(11)12)3-7(4)10(15)16/h2-3H,1H3

InChI Key: SPSSULHKWOKEEL-UHFFFAOYSA-N

Formula: C7H5N3O6

SMILES: Cc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-]

Molecular Weight: 227.13

CAS: 118-96-7

Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{solid}$	-3406.00 ± 3.00	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-3388.60 ± 3.00	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-3407.00	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-3404.50 ± 2.10	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-3401.80 ± 3.40	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-3402.30 ± 3.40	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-3419.18	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-3434.00	kJ/mol	NIST Webbook
$\Delta_f G°$	198.23	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	24.10 ± 3.50	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	-63.20 ± 5.00	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	-80.50 ± 3.10	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	-49.96	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	40.84	kJ/mol	Joback Method
$\Delta_{sub} H°$	113.20 ± 1.50	kJ/mol	NIST Webbook

Property	Value	Unit	Source
$\Delta_{sub}H°$	105.00 ± 2.00	kJ/mol	NIST Webbook
$\Delta_{sub}H°$	104.60 ± 1.70	kJ/mol	NIST Webbook
$\Delta_{sub}H°$	118.00	kJ/mol	NIST Webbook
$\Delta_{vap}H°$	87.00 ± 1.90	kJ/mol	NIST Webbook
IE	10.59 ± 0.04	eV	NIST Webbook
$logP_{oct/wat}$	1.720		Crippen Method
P_c	4067.32	kPa	Joback Method
T_{boil}	856.70	K	Joback Method
T_c	1146.44	K	Joback Method
T_{fus}	355.10 ± 0.10	K	NIST Webbook
T_{fus}	352.00 ± 0.10	K	NIST Webbook
T_{fus}	354.00 ± 2.00	K	NIST Webbook
T_{fus}	354.30 ± 0.50	K	NIST Webbook
T_{fus}	353.42 ± 0.30	K	NIST Webbook
V_c	0.566	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	371.64	J/mol×K	856.7	Joback Method
$C_{p,solid}$	311.70	J/mol×K	293.0	NIST Webbook
$C_{p,solid}$	243.30	J/mol×K	298.0	NIST Webbook
$\Delta_{fus}H$	23.43	kJ/mol	352.2	NIST Webbook
$\Delta_{fus}H$	23.40	kJ/mol	352.2	NIST Webbook
$\Delta_{fus}H$	23.43	kJ/mol	352.2	NIST Webbook
$\Delta_{sub}H$	99.00 ± 2.00	kJ/mol	313.5	NIST Webbook
$\Delta_{sub}H$	112.40	kJ/mol	323.0	NIST Webbook
$\Delta_{sub}H$	103.30 ± 2.50	kJ/mol	338.0	NIST Webbook

Property	Value	Unit	Temperature (K)	Source
$\Delta_{sub}H$	118.40 ± 4.20	kJ/mol	338.0	NIST Webbook
$\Delta_{vap}H$	93.70	kJ/mol	438.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H5N3O6/c1-4-6(9(13)14)2-5(8(11)12)3-7(4)10(15)16/h2-3H,1H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

Δ_c**H°**$_{solid}$: Standard solid enthalpy of combustion (kJ/mol).
C$_{p,gas}$: Ideal gas heat capacity (J/mol×K).
C$_{p,solid}$: Solid phase heat capacity (J/mol×K).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°**$_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
Δ_f**H°**$_{solid}$: Solid phase enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{fus}**H**: Enthalpy of fusion at a given temperature (kJ/mol).
Δ_{sub}**H°**: Enthalpy of sublimation at standard conditions (kJ/mol).
Δ_{sub}**H**: Enthalpy of sublimation at a given temperature (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
Δ_{vap}**H**: Enthalpy of vaporization at a given temperature (kJ/mol).
IE: Ionization energy (eV).
***log*P**$_{oct/wat}$: Octanol/Water partition coefficient .
P$_c$: Critical Pressure (kPa).
T$_{boil}$: Normal Boiling Point Temperature (K).
T$_c$: Critical Temperature (K).
T$_{fus}$: Normal melting (fusion) point (K).
V$_c$: Critical Volume (m^3/kg-mol).