2,4,6-TRINITRO-3-METHYLPHENOL

Other names:	2,4,6-Trinitro-m-cresol Phenol, 3-methyl-2,4,6-trinitro- m-Cresol, 2,4,6-trinitro- Cresylite Picric acid, methyl- Picric acid, 3-methyl- Trinitro-m-cresol Trinitro-m-cresolic acid 2,4,6-Trinitro-3-methylphenol Trinitro-meta-cresol UN 0216 3-Methylpicric acid Methylpicric acid NSC 3182
Inchi:	InChI=1S/C7H5N3O7/c1-3-4(8(12)13)2-5(9(14)15)7(11)6(3)10(16)17/h2,11H,1H3
InchiKey:	YYGJRRYSYLLCQH-UHFFFAOYSA-N
Formula:	C7H5N3O7
SMILES:	Cc1c([N+](=O)[O-])cc([N+](=O)[O-])c(O)c1[N+](=O)[O-]
Mol. weight [g/mol]:	243.13

Physical Properties

Property code	Value	Unit	Source
chs	-3212.70 ± 3.20	kJ/mol	NIST Webbook
chs	-3213.90 ± 3.20	kJ/mol	NIST Webbook
hf	-94.09	kJ/mol	Cheméo Relay (1.0)
hfus	46.63	kJ/mol	Joback Method
hsub	111.20 ± 2.10	kJ/mol	NIST Webbook
hsub	104.60	kJ/mol	NIST Webbook
hvap	85.12	kJ/mol	Cheméo Relay (1.0)
ie	9.63	eV	Cheméo Relay (1.0)
log10ws	-3.01		Cheméo Relay (1.0)
logp	1.425		Crippen Method
mcvol	143.860	ml/mol	McGowan Method
tb	538.67	K	Cheméo Relay (1.0)
tf	395.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.16	J/mol×K	937.32	Joback Method
cpg	411.79	J/mol×K	986.05	Joback Method
cpg	419.22	J/mol×K	1034.78	Joback Method
cpg	426.61	J/mol×K	1083.51	Joback Method
cpg	434.10	J/mol×K	1132.24	Joback Method
cpg	441.84	J/mol×K	1180.97	Joback Method
cpg	449.98	J/mol×K	1229.70	Joback Method
hsubt	103.30	kJ/mol	337.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C602993&Units=SI

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

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

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hsub: Enthalpy of sublimation at standard conditions

hsubt: Enthalpy of sublimation at a given temperature

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point