

2,4,6-TRINITRO-M-PHENYLENEDIAMINE

Other names:	m-Phenylenediamine, 2,4,6-trinitro-DATB 1,3-Diamino-2,4,6-trinitrobenzene 2,4-Diamino-1,3,5-trinitrobenzene 2,4,6-Trinitro-1,3-benzenediamine 2,4,6-trinitrobenzene-1,3-diamine
Inchi:	InChI=1S/C6H5N5O6/c7-4-2(9(12)13)1-3(10(14)15)5(8)6(4)11(16)17/h1H,7-8H2
InchiKey:	FZAZPMLWYUKRAE-UHFFFAOYSA-N
Formula:	C6H5N5O6
SMILES:	Nc1c([N+](=O)[O-])cc([N+](=O)[O-])c(N)c1[N+](=O)[O-]
Mol. weight [g/mol]:	243.14

Physical Properties

Property code	Value	Unit	Source
chs	-2978.00 ± 1.00	kJ/mol	NIST Webbook
chs	-2953.50	kJ/mol	NIST Webbook
hfs	-98.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-122.30	kJ/mol	NIST Webbook
hfus	48.26	kJ/mol	Joback Method
ie	8.90	eV	Cheméo Relay (1.0)
log10ws	-3.81		Cheméo Relay (1.0)
logp	0.576		Crippen Method
mcvol	143.860	ml/mol	McGowan Method
tb	587.28	K	Cheméo Relay (1.0)
tf	502.70	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.06	J/mol×K	983.86	Joback Method
cpg	412.18	J/mol×K	1033.66	Joback Method
cpg	416.42	J/mol×K	1083.47	Joback Method
cpg	419.82	J/mol×K	1133.27	Joback Method
cpg	422.43	J/mol×K	1183.08	Joback Method

cpg	424.32	J/mol×K	1232.88	Joback Method
cpg	425.51	J/mol×K	1282.68	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1630086&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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

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