1,3-Benzenediamine, 2,4,6-trinitro-

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]:	243.13
CAS:	1630-08-6

Physical Properties

Property code	Value	Unit	Source
chs	-2953.50	kJ/mol	NIST Webbook
chs	-2978.00 ± 1.00	kJ/mol	NIST Webbook
gf	313.08	kJ/mol	Joback Method
hf	58.78	kJ/mol	Joback Method
hfs	-122.30	kJ/mol	NIST Webbook
hfs	-98.00 ± 3.00	kJ/mol	NIST Webbook
hfus	48.26	kJ/mol	Joback Method
hvap	104.93	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	0.576		Crippen Method
mcvol	143.860	ml/mol	McGowan Method
pc	5304.68	kPa	Joback Method
tb	983.86	K	Joback Method
tc	1282.68	K	Joback Method
tf	831.23	K	Joback Method
vc	0.568	m3/kmol	Joback Method

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1630086&Units=SI&Mask=3FFF
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas 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
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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