1,3,5-Benzenetriamine, 2,4,6-trinitro-

Other names:	s-Triaminotrinitrobenzene
	sym-Triaminotrinitrobenzene
	TATB
	1,3,5-Triamino-2,4,6-trinitrobenzene
	2,4,6-Trinitro-1,3,5-benzenetriamine
	2,4,6-Trinitrobenzene-1,3,5-triamine
	NSC 243156
Inchi:	InChI=1S/C6H6N6O6/c7-1-4(10(13)14)2(8)6(12(17)18)3(9)5(1)11(15)16/h7-9H2
InchiKey:	JDFUJAMTCCQARF-UHFFFAOYSA-N
Formula:	C6H6N6O6
SMILES:	Nc1c([N+](=O)[O-])c(N)c([N+](=O)[O-])c(N)c1[N+](=O)[O-]
Mol. weight [g/mol]:	258.15
CAS:	3058-38-6

Physical Properties

Property code	Value	Unit	Source
chs	-3079.00 ± 2.00	kJ/mol	NIST Webbook
gf	369.90	kJ/mol	Joback Method
hf	81.10	kJ/mol	Joback Method
hfs	-74.70 ± 3.00	kJ/mol	NIST Webbook
hfs	-140.00 ± 5.00	kJ/mol	NIST Webbook
hfs	-154.00	kJ/mol	NIST Webbook
hfus	53.07	kJ/mol	Joback Method
hvap	116.23	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	0.158		Crippen Method
mcvol	153.840	ml/mol	McGowan Method
pc	5644.74	kPa	Joback Method
tb	1061.37	K	Joback Method
tc	1361.30	K	Joback Method
tf	927.01	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.99	J/mol×K	1061.37	Joback Method
cpg	452.00	J/mol×K	1111.36	Joback Method
cpg	455.08	J/mol×K	1161.35	Joback Method
cpg	457.27	J/mol×K	1211.34	Joback Method
cpg	458.62	J/mol×K	1261.32	Joback Method
cpg	459.16	J/mol×K	1311.31	Joback Method
cpg	458.93	J/mol×K	1361.30	Joback Method
hsubt	168.00	kJ/mol	423.00	NIST Webbook
hsubt	168.20	kJ/mol	426.50	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3058386&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hsubt: Enthalpy of sublimation at a given temperature
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