1,3,5-Trinitrobenzene

Other names:	1,3,5-trinitrobenzene [1,3,5-TNB]
	Benzene,1,3,5-trinitro-
	NSC 36931
	Rcra waste number U234
	TNB
	Trinitrobenzeen
	Trinitrobenzene
	Trinitrobenzol
	s-Trinitrobenzene
	sym-Trinitrobenzene
	syn-Trinitrobenzene
Inchi:	InChI=1S/C6H3N3O6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H
InchiKey:	UATJOMSPNYCXIX-UHFFFAOYSA-N
Formula:	C6H3N3O6
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	213.10
CAS:	99-35-4

Physical Properties

Property code	Value	Unit	Source
chs	-2746.80 ± 2.80	kJ/mol	NIST Webbook
chs	-2785.00	kJ/mol	NIST Webbook
chs	-2753.00 ± 0.40	kJ/mol	NIST Webbook
chs	-2745.90 ± 2.80	kJ/mol	NIST Webbook
ea	2.63	eV	NIST Webbook
gf	199.44	kJ/mol	Joback Method
hf	14.14	kJ/mol	Joback Method
hfs	-37.00 ± 1.00	kJ/mol	NIST Webbook
hfus	38.64	kJ/mol	Joback Method
hsub	107.30 ± 0.60	kJ/mol	NIST Webbook
hvap	82.32	kJ/mol	Joback Method
ie	10.96 ± 0.02	eV	NIST Webbook
log10ws	-2.89		Aqueous Solubility Prediction Method
log10ws	-2.89		Estimated Solubility Method
logp	1.411		Crippen Method

mcvol	123.900	ml/mol	McGowan Method
pc	4710.65	kPa	Joback Method
rinpol	285.91		NIST Webbook
rinpol	287.18		NIST Webbook
rinpol	284.47		NIST Webbook
rinpol	284.47		NIST Webbook
tb	828.84	K	Joback Method
tc	1125.82	K	Joback Method
tf	398.40 ± 1.00	K	NIST Webbook
tf	397.70 ± 1.00	K	NIST Webbook
tf	396.15 ± 1.00	K	NIST Webbook
tf	394.20 ± 0.10	K	NIST Webbook
tf	394.65	K	Aqueous Solubility Prediction Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.12	J/mol×K	1125.82	Joback Method
cpg	345.27	J/mol×K	1026.83	Joback Method
cpg	349.01	J/mol×K	1076.33	Joback Method
cpg	322.71	J/mol×K	828.84	Joback Method
cpg	329.63	J/mol×K	878.34	Joback Method
cpg	335.65	J/mol×K	927.83	Joback Method
cpg	340.84	J/mol×K	977.33	Joback Method
cps	222.70	J/mol×K	298.15	NIST Webbook
cps	214.60	J/mol×K	298.15	NIST Webbook
hfust	14.80	kJ/mol	380.30	NIST Webbook
hfust	14.81	kJ/mol	380.30	NIST Webbook
hfust	1.90	kJ/mol	370.00	NIST Webbook
hvapt	70.30	kJ/mol	530.00	NIST Webbook
sfust	38.95	J/mol×K	380.30	NIST Webbook
sfust	5.13	J/mol×K	370.00	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.34627e+01
Coeff. B	-1.50053e+04
Coeff. C	1.70052e+02
Temperature range (K), min.	477.42
Temperature range (K), max.	656.63

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.23638e+01
Coeff. B	-1.03546e+04
Coeff. C	-3.61178e+00
Coeff. D	-2.01475e-09
Temperature range (K), min.	398.40
Temperature range (K), max.	748.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99354&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1436
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility of 4-Nitrotoluene, 2,6-Dinitrotoluene, 2,3-Dinitrotoluene, and 1,3,5-Trinitrobenzene in Pure Water and Seawater:	https://www.doi.org/10.1021/je700374j
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1436

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ea:	Electron affinity

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume