Benzene, 2-chloro-1,3,5-trinitro-

Other names:	1-Chloro-2,4,6-trinitrobenzene
	2,4,6-Trinitro-1-chlorobenzene
	2,4,6-Trinitrochlorobenzene
	2-Chloro-1,3,5-trinitrobenzene
	Picryl chloride
	Tncb
Inchi:	InChI=1S/C6H2ClN3O6/c7-6-4(9(13)14)1-3(8(11)12)2-5(6)10(15)16/h1-2H
InchiKey:	HJRJRUMKQCMYDL-UHFFFAOYSA-N
Formula:	C6H2ClN3O6
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])c(Cl)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	247.55
CAS:	88-88-0

Physical Properties

Property code	Value	Unit	Source
chs	-2691.16	kJ/mol	NIST Webbook
gf	177.88	kJ/mol	Joback Method
hf	-13.07	kJ/mol	Joback Method
hfs	20.80	kJ/mol	NIST Webbook
hfus	42.45	kJ/mol	Joback Method
hvap	87.37	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	2.065		Crippen Method
mcvol	136.140	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
tb	871.25	K	Joback Method
tc	1168.90	K	Joback Method
tf	682.11	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.08	J/mol×K	1119.29	Joback Method

cpg	334.86	J/mol×K	871.25	Joback Method
cpg	340.65	J/mol×K	920.86	Joback Method
cpg	345.61	J/mol×K	970.47	Joback Method
cpg	349.79	J/mol×K	1020.08	Joback Method
cpg	353.27	J/mol×K	1069.69	Joback Method
cpg	358.30	J/mol×K	1168.90	Joback Method
hvapt	63.10	kJ/mol	508.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63366e+01
Coeff. B	-7.59393e+03
Temperature range (K), min.	473.00
Temperature range (K), max.	688.78

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C88880&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume