Benzene, 1,3,5-trichloro-2,4,6-trinitro-

Other names:	1,3,5-Trichloro-2,4,6-Trinitrobenzene
	1,3,5-trichlorotrinitrobenzene
	Bulbosan
	TCTNB
	Trichloro-1,3,5-Trinitrobenzene
	sym-Trichlorotrinitrobenzene
Inchi:	InChI=1S/C6Cl3N3O6/c7-1-4(10(13)14)2(8)6(12(17)18)3(9)5(1)11(15)16
InchiKey:	LZMONXBJUOXABQ-UHFFFAOYSA-N
Formula:	C6Cl3N3O6
SMILES:	O=[N+]([O-])c1c(Cl)c([N+](=O)[O-])c(Cl)c([N+](=O)[O-])c1Cl
Mol. weight [g/mol]:	316.44
CAS:	2631-68-7

Physical Properties

Property code	Value	Unit	Source
gf	134.76	kJ/mol	Joback Method
hf	-67.49	kJ/mol	Joback Method
hfus	50.07	kJ/mol	Joback Method
hvap	97.46	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	3.371		Crippen Method
mcvol	160.620	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
tb	956.07	K	Joback Method
tc	1254.68	K	Joback Method
tf	766.99	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.34	J/mol×K	956.07	Joback Method
cpg	359.05	J/mol×K	1005.84	Joback Method
cpg	362.01	J/mol×K	1055.61	Joback Method

cpg	364.25	J/mol×K	1105.37	Joback Method
cpg	365.82	J/mol×K	1155.14	Joback Method
cpg	366.74	J/mol×K	1204.91	Joback Method
cpg	367.06	J/mol×K	1254.68	Joback Method
hvapt	68.90	kJ/mol	523.00	NIST Webbook
hvapt	43.20	kJ/mol	523.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.86130e+01
Coeff. B	-8.29322e+03
Temperature range (K), min.	452.55
Temperature range (K), max.	623.48

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2631687&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

Legend

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: 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