Benzene, 1,2,4,5-tetrachloro-3-nitro-

Other names:	Chipman 3,142
	Folosan
	Folosan DB-905
	Fusarex
	Myfusan
	Tecnazen
	Tetrachloronitrobenzene
	TCNB
	1,2,4,5-Tetrachloro-3-Nitrobenzene
	2,3,5,6-Tetrachloro-1-nitrobenzene
	2,3,5,6-Tetrachloronitrobenzene
	Benzene, 3-nitro-1,2,4,5-tetrachloro-
	2,3,5,6-Tetrachlor-3-nitrobenzol
	DB 905
	Teknazen
	Chipman 3142
	Napotate
	Nebulin
	Arena
	Bygran
	Easytec
	Hickstor
	Hystore
	Hytec
	New Hystor
	Tecnazene
	Turbostore
	1-Nitro-2,3,5,6-tetrachlorobenzene
Inchi:	InChI=1S/C6HCl4NO2/c7-2-1-3(8)5(10)6(4(2)9)11(12)13/h1H
InchiKey:	XQTLDIFVVHJORV-UHFFFAOYSA-N
Formula:	C6HCl4NO2
SMILES:	O=[N+]([O-])c1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	260.89
CAS:	117-18-0

Physical Properties

Property code	Value	Unit	Source

gf	61.36	kJ/mol	Joback Method
hf	-50.24	kJ/mol	Joback Method
hfus	31.93	kJ/mol	Joback Method
hsub	91.30 ± 2.50	kJ/mol	NIST Webbook
hvap	68.00	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.208		Crippen Method
mcvol	138.020	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	1594.00		NIST Webbook
tb	577.20	K	NIST Webbook
tc	956.14	K	Joback Method
tf	373.55 ± 0.20	K	NIST Webbook
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.02	J/mol×K	684.84	Joback Method
cpg	253.77	J/mol×K	730.06	Joback Method
cpg	258.97	J/mol×K	775.27	Joback Method
cpg	263.65	J/mol×K	820.49	Joback Method
cpg	267.82	J/mol×K	865.71	Joback Method
cpg	271.52	J/mol×K	910.92	Joback Method
cpg	274.77	J/mol×K	956.14	Joback Method
hfust	19.46	kJ/mol	373.30	NIST Webbook
hfust	19.46	kJ/mol	373.30	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C117180&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume