Tetrachloroisophthalonitrile

Other names:

1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro-
1,3-Dicyano-2,4,5,6-tetrachlorobenzene
1,3-Dicyanotetrachlorobenzene
2,4,5,6-Tetrachloro-1,3-benzenedicarbonitrile
2,4,5,6-Tetrachloro-1,3-dicyanobenzene
2,4,5,6-Tetrachloro-1,3-isophthalonitrile
2,4,5,6-Tetrachloro-3-cyanobenzonitrile
2,4,5,6-Tetrachloroisophthalonitrile
2,4,5,6-tetrachlorobenzene-1,3-dicarbonitrile
Benzenedicarbonitrile, 2,4,5,6-tetrachloro-
Bravo
Bravo 500
Bravo 6F
Bravo 720
Bravo Ultrex
Bravo-W-75
Chloroalonil
Chlorothalonil
Chlorthalonil
Clortosip
DAC 2787
Daconil
Daconil 1000
Daconil 2787
Daconil 2787 flowable fungicide
Daconil M
Dacosoil
Dakoflo
Exotherm
Exotherm termil
Faber
Forturf
Hortyl
Isophthalonitrile, 2,4,5,6-tetrachloro-
Isophthalonitrile, tetrachloro-
NCI-C00102
Nopcocide
Nopcocide N 96
Nopcocide N40D & N96
Repulse

	Siclor
	Sweep
	TPN
	Termil
	Tetrachlorisoftalonitril
	Tetrachloro-1,3-dicyanobenzene
	Tetrachloro-m-phthalodinitrile
	Tetrachlorobenzene-1,3-dicarbonitrile
	Tetrachloroisophthalodinitrile
	Thalonil
	Tpn (pesticide)
	Tripart faber
	Tripart ultrafaber
	Vanox
	m-TCPN
	m-Tetrachlorophthalodinitrile
	m-Tetrachlorophthalonitrile
	meta-Tetrachlorophthalodinitrile
Inchi:	InChI=1S/C8Cl4N2/c9-5-3(1-13)6(10)8(12)7(11)4(5)2-14
InchiKey:	CRQQGFGUEAVUIL-UHFFFAOYSA-N
Formula:	C8Cl4N2
SMILES:	N#Cc1c(Cl)c(Cl)c(Cl)c(C#N)c1Cl
Mol. weight [g/mol]:	265.91
CAS:	1897-45-6

Physical Properties

Property code	Value	Unit	Source
chs	-3436.70 ± 2.20	kJ/mol	NIST Webbook
gf	299.38	kJ/mol	Joback Method
hf	237.53	kJ/mol	Joback Method
hfs	189.60 ± 4.60	kJ/mol	NIST Webbook
hfus	28.37	kJ/mol	Joback Method
hvap	77.48	kJ/mol	Joback Method
log10ws	-5.64		Estimated Solubility Method
log10ws	-4.91		Aqueous Solubility Prediction Method
logp	4.044		Crippen Method
mcvol	151.540	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method

rinpol	1795.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1829.00		NIST Webbook
tb	787.90	K	Joback Method
tc	1048.40	K	Joback Method
tf	526.20 ± 0.20	K	NIST Webbook
tf	526.72 ± 0.20	K	NIST Webbook
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.96	J/mol×K	787.90	Joback Method
cpg	272.09	J/mol×K	831.32	Joback Method
cpg	275.82	J/mol×K	874.73	Joback Method
cpg	279.15	J/mol×K	918.15	Joback Method
cpg	282.09	J/mol×K	961.57	Joback Method
cpg	284.64	J/mol×K	1004.98	Joback Method
cpg	286.81	J/mol×K	1048.40	Joback Method
hfust	30.00	kJ/mol	526.20	NIST Webbook
hsubt	109.10	kJ/mol	390.50	NIST Webbook
hvapt	67.00	kJ/mol	388.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1897456&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solubility of Organic Biocides in Supercritical CO2 and CO2 + Cosolvent Mixtures: https://www.doi.org/10.1021/je0255473

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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