

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

Other names:	1-Nitro-2,3,4,5-tetrachlorobenzene 1,2,3,4-Tetrachloro-5-nitrobenzene 2,3,4,5-Tetrachloro-1-nitrobenzene 2,3,4,5-Tetrachloronitrobenzene Benzene, 5-nitro-1,2,3,4-tetrachloro- DB-905 Folosan DB-905 fumite TCBN NSC 5577 NSC 57752
Inchi:	InChI=1S/C6HCl4NO2/c7-2-1-3(11(12)13)5(9)6(10)4(2)8/h1H
InchiKey:	MTBYTWZDRVOMBR-UHFFFAOYSA-N
Formula:	C6HCl4NO2
SMILES:	O=[N+](O-)[c]1cc(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	260.89
CAS:	879-39-0

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
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
tb	684.84	K	Joback Method
tc	956.14	K	Joback Method
tf	497.17	K	Joback Method
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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C879390&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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