Benzene, pentachloronitro-

Other names:

Avicol
Avicol, pesticide
Batrilex
Benzene, 1,2,3,4,5-pentachloro-6-nitro-
Botrilex
Brassicol
Brassicol 75
Brassicol Super
Chinozan
Earthcide
Fartox
Folosan
Fomac 2
Fungiclor
GC 3944-3-4
KOBU
KP 2
Kobutol
Liro-PCNB
Marisan forte
NCI-C00419
Nitropentachlorobenzene
Olpisan
PCNB
PKHNB
Pentachlornitrobenzol
Pentachloronitrobenzene
Pentachloronitrobenzol
Pentagen
Phomasan
Quinosan
Quintocene
Quintozen
Quintozene
RTU 1010
Saniclor 30
Terrachlor
Terraclor
Terraclor 30 G
Terrafun

	Terrazan
	Tilcarex
	Tritisan
Inchi:	InChI=1S/C6Cl5NO2/c7-1-2(8)4(10)6(12(13)14)5(11)3(1)9
InchiKey:	LKPLKUMXSAEKID-UHFFFAOYSA-N
Formula:	C6Cl5NO2
SMILES:	O=[N+]([O-])c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	295.33
CAS:	82-68-8

Physical Properties

Property code	Value	Unit	Source
gf	39.80	kJ/mol	Joback Method
hf	-77.45	kJ/mol	Joback Method
hfus	35.74	kJ/mol	Joback Method
hsub	96.30 ± 2.10	kJ/mol	NIST Webbook
hsub	94.50 ± 0.40	kJ/mol	NIST Webbook
hvap	73.05	kJ/mol	Joback Method
log10ws	-5.82		Estimated Solubility Method
log10ws	-5.82		Aqueous Solubility Prediction Method
logp	4.862		Crippen Method
mcvol	150.260	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	1754.00		NIST Webbook
rinpol	297.93		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	298.71		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1798.00		NIST Webbook
rinpol	1771.00		NIST Webbook
rinpol	1754.00		NIST Webbook
ripol	2355.00		NIST Webbook
tb	727.25	K	Joback Method
tc	1001.02	K	Joback Method
tf	417.58 ± 0.20	K	NIST Webbook
tf	418.00 ± 0.20	K	NIST Webbook

tf	415.90	K	Aqueous Solubility Prediction Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.26	J/mol×K	955.40	Joback Method
cpg	260.84	J/mol×K	727.25	Joback Method
cpg	265.69	J/mol×K	772.88	Joback Method
cpg	270.04	J/mol×K	818.51	Joback Method
cpg	273.90	J/mol×K	864.14	Joback Method
cpg	277.31	J/mol×K	909.77	Joback Method
cpg	282.78	J/mol×K	1001.02	Joback Method
hfust	18.41	kJ/mol	418.00	NIST Webbook
hsubt	93.00 ± 0.40	kJ/mol	328.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C82688&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
hsubt: Enthalpy of sublimation at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume