Heptachlor

Other names:

1(3a),4,5,6,7,8,8-Heptachloro-3a(1),4,7,7a-tetrahydro-4,7-methanoindene
1,4,5,6,7,10,10-Heptachloro-4,7,8,9-tetrahydro-4,7-endo-methyleneindene
1,4,5,6,7,10,10-Heptachloro-4,7,8,9-tetrahydro-4,7-methyleneindene
1,4,5,6,7,8,8-Eptacloro-3a,4,7,7a-tetraidro-4,7-endo-metano-indene
1,4,5,6,7,8,8-Heptachloor-3a,4,7,7a-tetrahydro-4,7-endo-methano-indeen
1,4,5,6,7,8,8-Heptachlor-3a,4,7,7,7a-tetrahydro-4,7-endo-methano-inden
1,4,5,6,7,8,8-Heptachloro-3a,4,7,7,7a-tetrahydro-4,7-methylene indene
1,4,5,6,7,8,8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-endo-methanoindene
1,4,5,6,7,8,8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-endomethanoindene (heptachlor)
1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-4,7-methanoindene
1,4,5,6,7,8,8a-Heptachloro-3a,4,7,7a-tetrahydro-4,7-methanoindane
3,4,5,6,7,8,8a-Heptachlorodicyclopentadiene
3-Chlorochlordene
3a,4,5,6,7,8,8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-methanoindene
4,7-Methano-1H-indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-
4,7-Methanoindene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-
Aahepta
Agroceres
Arbinex 30TN
Dicyclopentadiene, 3,4,5,6,7,8,8a-heptachloro-
Drinox H-34
E 3314
ENT 15,152
Eptacloro
GPKh
H-34
H-60
Hepta
Heptachloor
Heptachlorane
Heptachlore
Heptachlorotetrahydro-4,7-methanoindene
Heptagran
Heptamul
Heptox
Latka 104
NCI-C00180
NSC 8930
Rcra waste number P059
Rhodiachlor

	Technical heptachlor
	Velsicol 104
	Velsicol heptachlor
Inchi:	InChI=1S/C10H5Cl7/c11-4-2-1-3-5(4)9(15)7(13)6(12)8(3,14)10(9,16)17/h1-5H
InchiKey:	FRCCEHPWNOQAEU-UHFFFAOYSA-N
Formula:	C10H5Cl7
SMILES:	ClC1=C(Cl)C2(Cl)C3C(Cl)C=CC3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]:	373.32
CAS:	76-44-8

Physical Properties

Property code	Value	Unit	Source
gf	121.02	kJ/mol	Joback Method
hf	-70.35	kJ/mol	Joback Method
hfus	29.33	kJ/mol	Joback Method
hvap	65.99	kJ/mol	Joback Method
log10ws	-6.32		Estimated Solubility Method
logp	5.242		Crippen Method
mcvol	196.260	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1861.00		NIST Webbook
rinpol	1863.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1861.00		NIST Webbook
rinpol	1863.00		NIST Webbook
rinpol	1866.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1891.00		NIST Webbook
rinpol	1860.70		NIST Webbook
rinpol	1886.10		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1922.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1890.00		NIST Webbook

rinpol	1880.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1861.00		NIST Webbook
rinpol	1863.00		NIST Webbook
rinpol	1889.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1920.00		NIST Webbook
ripol	2484.00		NIST Webbook
ripol	2505.00		NIST Webbook
ripol	2505.00		NIST Webbook
tb	709.69	K	Joback Method
tc	988.83	K	Joback Method
tf	366.00 ± 1.00	K	NIST Webbook
tf	369.00 ± 0.20	K	NIST Webbook
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.08	J/mol×K	942.31	Joback Method
cpg	413.85	J/mol×K	709.69	Joback Method
cpg	424.00	J/mol×K	756.21	Joback Method
cpg	434.97	J/mol×K	802.74	Joback Method
cpg	447.49	J/mol×K	849.26	Joback Method
cpg	462.28	J/mol×K	895.78	Joback Method
cpg	501.60	J/mol×K	988.83	Joback Method
hfust	20.72	kJ/mol	362.20	NIST Webbook
hfust	2.09	kJ/mol	371.00	NIST Webbook
hvapt	76.50	kJ/mol	398.00	NIST Webbook

Sources

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

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=C76448&Units=SI

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
hfust:	Enthalpy of fusion 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume