

trans-Chlordane

Other names:	(1«alpha»,2«beta»,3a«alpha»,4«beta»,7«beta»,7a«alpha»)-1,2,4,5,6,7,8,8-octachloro-2,3,4,7,7a-hexahydro-1H-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-, (1R,2R,3aS,4S,7R,7aS)-rel-4,7-Methano-1H-Indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-, (1«alpha»,2«beta»,3a«alpha»,4«beta»,7«beta»,7a«alpha»)-4,7-Methano-1H-Indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-, (1Â«alphaÂ»,2Â«betaÂ»,3aÂ«alphaÂ»,4Â«betaÂ»,7Â«betaÂ»,7aÂ«alphaÂ»)-4,7-Methanoindan, 1«beta»,2«alpha»,4«alpha»,5,6,7«alpha»,8,8-octachloro-3a«beta»,4,7,7a«beta»-tetrahydro-4,7-Methanoindan, 1Â«betaÂ»,2Â«alphaÂ»,4Â«alphaÂ»,5,6,7Â«alphaÂ»,8,8-octachloro-3aÂ«betaÂ»,4,7,7aÂ«betaÂ»-tetrahydro-4,7-Methanoindan, 3a-«beta»,4,7,7a-«beta»-tetrahydro-1-«beta»,2-«alpha»,4-«alpha»,5,6,7-«alpha»,8,8-octachloro-3a-«beta»,4,7,7a-Â«betaÂ»-tetrahydro-1-Â«betaÂ»,2-Â«alphaÂ»,4-Â«alphaÂ»,5,6,7-Â«betaÂ»-Chlordan, trans-Chlordane «gamma» (trans) Chlordane Â«gammaÂ» (trans) Chlordane, trans-trans-Chlordan trans-«gamma»-Chlordane trans-Â«gammaÂ»-Chlordane «beta»-Chlordan «beta»-Chlordane Â«betaÂ»-Chlordan Â«betaÂ»-Chlordane
Inchi:	InChI=1S/C10H6Cl8/c11-3-1-2-4(5(3)12)9(16)7(14)6(13)8(2,15)10(9,17)18/h2-5H,1H2/t2
InchiKey:	BIWJNBZANLAXMG-SVSLFMFOSA-N
Formula:	C10H6Cl8
SMILES:	C1C1=C(Cl)C2(Cl)C3C(Cl)C(Cl)CC3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]:	409.78
CAS:	5103-74-2

Physical Properties

Property code	Value	Unit	Source
gf	71.42	kJ/mol	Joback Method
hf	-164.21	kJ/mol	Joback Method
hfus	33.37	kJ/mol	Joback Method
hvap	69.77	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.683		Crippen Method
mcvol	212.800	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method

rinpol	2021.00		NIST Webbook
rinpol	2021.00		NIST Webbook
rinpol	2089.00		NIST Webbook
ripol	2829.00		NIST Webbook
tb	743.29	K	Joback Method
tc	1021.42	K	Joback Method
tf	572.66	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.76	J/mol×K	928.71	Joback Method
cpg	540.74	J/mol×K	975.06	Joback Method
cpg	461.86	J/mol×K	743.29	Joback Method
cpg	473.85	J/mol×K	789.64	Joback Method
cpg	487.02	J/mol×K	836.00	Joback Method
cpg	502.09	J/mol×K	882.35	Joback Method
cpg	565.73	J/mol×K	1021.42	Joback Method
hvapt	81.70	kJ/mol	391.00	NIST Webbook
hvapt	80.70	kJ/mol	398.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.12705e+01
Coeff. B	-5.16209e+03
Coeff. C	1.03890e+01
Temperature range (K), min.	459.62
Temperature range (K), max.	855.87

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=C5103742&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
pvap:	Vapor 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

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