Heptachlor epoxide

Other names:	2,5-Methano-2H-indeno[1,2-b]oxirene, 2,3,4,5,6,7,7-heptachloro-1a,1b,5,5a,6,6a-hexahydro-, (1aα,1bβ,2α,5α,5aβ,6β,6aα)-
	4,7-Methanoindan, 1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-
	Epoxyheptachlor
	ENT 25,584
	HCE
	Velsicol 53-CS-17
	1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-4,7-methanoindane
	2,5-Methano-2H-indeno[1,2-b]oxirene, 2,3,4,5,6,7,7-heptachloro-1a,1b,5,5a,6,6a-hexahydro-,(1aR,1bS,2R,5S,5aR,6S,6aR)-rel-
	Heptachlore epoxide
Inchi:	InChI=1S/C10H5Cl7O/c11-3-1-2(4-5(3)18-4)9(15)7(13)6(12)8(1,14)10(9,16)17/h1-5H
InchiKey:	ZXFXBSWRVIQKOD-UHFFFAOYSA-N
Formula:	C10H5Cl7O
SMILES:	ClC1=C(Cl)C2(Cl)C3C4OC4C(Cl)C3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]:	389.32
CAS:	66240-71-9

Physical Properties

Property code	Value	Unit	Source
gf	82.18	kJ/mol	Joback Method
hf	-195.35	kJ/mol	Joback Method
hfus	39.49	kJ/mol	Joback Method
hvap	69.47	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.453		Crippen Method
mcvol	195.570	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	1993.00		NIST Webbook
rinpol	1997.00		NIST Webbook
rinpol	2023.00		NIST Webbook
rinpol	2040.00		NIST Webbook
rinpol	2015.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1997.00		NIST Webbook
rinpol	1999.00		NIST Webbook
rinpol	2002.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1997.00		NIST Webbook

rinpol	1999.00		NIST Webbook
rinpol	2003.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2072.00		NIST Webbook
rinpol	2015.00		NIST Webbook
rinpol	2023.00		NIST Webbook
ripol	2805.00		NIST Webbook
tb	731.01	K	Joback Method
tc	1003.31	K	Joback Method
tf	594.29	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.71	J/mol×K	731.01	Joback Method
cpg	457.39	J/mol×K	776.39	Joback Method
cpg	469.23	J/mol×K	821.78	Joback Method
cpg	482.96	J/mol×K	867.16	Joback Method
cpg	499.33	J/mol×K	912.54	Joback Method
cpg	519.09	J/mol×K	957.93	Joback Method
cpg	542.97	J/mol×K	1003.31	Joback Method

Sources

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=C66240719&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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