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
	1,4,5,6,7,8,8-Heptachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-4,7-endo-methanoindan
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:	1024-57-3

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	2012.00		NIST Webbook
rinpol	2015.00		NIST Webbook
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
ripol	2828.00		NIST Webbook
ripol	2828.00		NIST Webbook
ripol	2828.00		NIST Webbook
tb	731.01	K	Joback Method
tc	1003.31	K	Joback Method
tf	436.00 ± 0.20	K	NIST Webbook

tf	439.00 ± 1.00	K	NIST Webbook
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
hfust	2.85	kJ/mol	434.90	NIST Webbook
hvapt	75.00	kJ/mol	398.00	NIST Webbook

Sources

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=C1024573&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