

Endrin

Other names:	1,2,3,4,10,10-Hexachloro-6,7-Epoxy-1,4,4a,5,6,7,8,8a-octahydro-exo-1,4-exo-5,8-dimethan-1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-1,4-endo,endo-5,8-dimethan-1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-endo-1,4-endo-5,8-dimethan-1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-, endo,endo-2,7:3,6-Dimethanonaphth[2,3-b]oxirane, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, 6a«alpha»,2«beta»,2a«beta»,3«alpha»,6«alpha»,6a«beta»,7«beta»,7a«alpha»)-3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-2,7:3,6-dimethanonaphth(2,3-b)ox(1aA«alphaA»,2A«betaA»,2aA«betaA»,3A«alphaA»,6A«alphaA»,6aA«betaA»,7A«betaA» Cmpd. 269 Compd. 269 Compound 269 EN 57 ENT 17,251 Endrex Endricol Endrin isomer Endrin mixture Endrine Experimental Insecticide 269 Hexachloroepoxyoctahydro-endo,endo-dimethanonaphthalene Hexadrin Latka 269 Mendrin NA 2761 NCI-C00157 Nendrin OMS 197 Oktanex Rcra waste number P051 SD 3419 SD 3419 Illoxol
Inchi:	InChI=1S/C12H8Cl6O/c13-8-9(14)11(16)5-3-1-2(6-7(3)19-6)4(5)10(8,15)12(11,17)18/h2-
InchiKey:	DFBKLUNHFCTMDC-GKRDHZSOSA-N
Formula:	C12H8Cl6O
SMILES:	C1C1=C(Cl)C2(Cl)C3C4CC(C5OC45)C3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]:	380.91
CAS:	72-20-8

Physical Properties

Property code	Value	Unit	Source
gf	183.80	kJ/mol	Joback Method
hf	-141.93	kJ/mol	Joback Method
hfus	40.71	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-6.18		Estimated Solubility Method
logp	4.481		Crippen Method
mcvol	200.650	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	2157.00		NIST Webbook
rinpol	2183.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2183.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2200.00		NIST Webbook
ripol	3013.00		NIST Webbook
ripol	3013.00		NIST Webbook
tb	741.81	K	Joback Method
tc	1008.70	K	Joback Method
tf	608.37	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.75	J/mol×K	741.81	Joback Method
cpg	520.79	J/mol×K	786.29	Joback Method
cpg	535.04	J/mol×K	830.77	Joback Method
cpg	551.26	J/mol×K	875.26	Joback Method
cpg	570.24	J/mol×K	919.74	Joback Method
cpg	592.75	J/mol×K	964.22	Joback Method
cpg	619.56	J/mol×K	1008.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C72208&Units=SI

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

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