Dieldrin

Other names:

(1R,4S,4aS,5R,6R,7S,8S,8aR)-1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-oct
1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-1,4-endo,exo-5,8-dimeth
1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-1,4-endo-exo-5,8-dimeth
1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-endo,exo-1,4:5,8-dimeth
(dieldrin)
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,exo-
2,7:3,6-Dimethanonaphth(2,3-b)oxirene,
3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-,
2,7:3,6-Dimethanonaphth[2,3-b]oxirene,
3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-,
(1aR,2R,2aS,3S,6R,6aR,7S,7aS)-rel-
2,7:3,6-Dimethanonaphth[2,3-b]oxirene,
3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-,
(1a«alpha»,2«beta»,2a«alpha»,3«beta»,6«beta»,6a«alpha»,7«beta»,7a«alpha»)-
Aldrin epoxide
(1aÂ«alphaÂ»,2Â«betaÂ»,2aÂ«alphaÂ»,3Â«betaÂ»,6Â«betaÂ»,6aÂ«alphaÂ»,7Â«betaÂ
Alvit
Alvit 55
Compd. 497
Compound 497
Deildrin
Dieldrex
Dieldrine
Dieldrite
Dielmoth
Dildrin
Dorytox
ENT 16,225
ENT-16225
HEOD
Hexachloroepoxyoctahydro-endo,exo-dimethanonaphthalene
Illoxol
Insectlack
Kombi-Albertan
Mixture containing 85 percent of
1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-1,4-exo-5,8-endo-dimeth
Moth Snub D
NCI-C00124
Octalox
Panoram D-31
Red Shield
SD 3417
Shelltox
Termitox
exo-Dieldrin

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-NLUYNBKHSA-N

Formula: C12H8Cl6O

SMILES: ClC1=C(Cl)C2(Cl)C3C4CC(C5OC45)C3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]: 380.91
CAS: 60-57-1

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	-6.29		Estimated Solubility Method
logp	4.481		Crippen Method
mcvol	200.650	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	2137.00		NIST Webbook
rinpol	2159.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2107.00		NIST Webbook
rinpol	2111.00		NIST Webbook
rinpol	2114.00		NIST Webbook
rinpol	2108.00		NIST Webbook
rinpol	2111.00		NIST Webbook
rinpol	2114.00		NIST Webbook
rinpol	2110.45		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2118.88		NIST Webbook
rinpol	2125.66		NIST Webbook
rinpol	2120.14		NIST Webbook
rinpol	2132.97		NIST Webbook
rinpol	2127.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2109.00		NIST Webbook
rinpol	2139.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2139.00		NIST Webbook
rinpol	2110.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2175.00		NIST Webbook

rinpol	2107.00		NIST Webbook
rinpol	2114.00		NIST Webbook
rinpol	2112.80		NIST Webbook
rinpol	2132.35		NIST Webbook
rinpol	2120.14		NIST Webbook
ripol	3103.00		NIST Webbook
ripol	3103.00		NIST Webbook
tb	741.81	K	Joback Method
tc	1008.70	K	Joback Method
tf	448.00 ± 1.00	K	NIST Webbook
tf	453.00 ± 1.00	K	NIST Webbook
tf	452.00 ± 0.20	K	NIST Webbook
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.75	J/mol×K	964.22	Joback Method
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	619.56	J/mol×K	1008.70	Joback Method
hfust	3.04	kJ/mol	452.90	NIST Webbook
hsubt	93.80	kJ/mol	328.00	NIST Webbook
hsubt	98.70	kJ/mol	303.00	NIST Webbook
hvapt	82.50	kJ/mol	398.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60571&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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
hsubt:	Enthalpy of sublimation 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