Photodieldrin

Other names: 2,4,6-Metheno-2H-cyclopenta[4,5]pentaleno[1,2-b]oxirene, 2a,3,3,4,5,5a-hexachlorodecahydro-, (1aα,1bβ,2α,2aβ,4β,5β,5aβ,5bβ,6α)-; 2,4,7-Metheno-1H-cyclopenta[a]pentalene, 1,1a,2,3,3a,7a-hexachloro-5,6-epoxydecahydro-, stereoisomer

BL 6623

Dieldrin, photo-

NCI-C00599

Dieldrin photo derivative

Inchi: InChI=1S/C12H8Cl6O/c13-8-9(14)3-1-4-5(2(3)7-6(1)19-7)11(9,16)12(17,18)10(4,8)15/h1

InchiKey: LOVDWMTZZYUFMA-UHFFFAOYSA-N

Formula: C12H8Cl6O

SMILES: ClC1C2(Cl)C3C4C5OC5C5C4C1(Cl)C(Cl)(C53)C2(Cl)Cl

Mol. weight [g/mol]: 380.91

CAS: 13366-73-9

Physical Properties

Property code	Value	Unit	Source
gf	249.24	kJ/mol	Joback Method
hf	-110.93	kJ/mol	Joback Method
hfus	40.54	kJ/mol	Joback Method
hvap	65.29	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.617		Crippen Method
mcvol	194.090	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
tb	717.52	K	Joback Method
tc	983.44	K	Joback Method
tf	626.49	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.55	J/mol×K	717.52	Joback Method
cpg	528.33	J/mol×K	761.84	Joback Method
cpg	542.51	J/mol×K	806.16	Joback Method

cpg	559.11	J/mol×K	850.48	Joback Method
cpg	579.14	J/mol×K	894.80	Joback Method
cpg	603.63	J/mol×K	939.12	Joback Method
cpg	633.57	J/mol×K	983.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13366739&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume