

Endrin ketone

Other names:	2,5,7-Metheno-3H-cyclopenta[a]pentalen-3-one, 3b,4,5,6,6a-hexachlorodecahydro-, «delta»-Ketoendrin (2«alpha»,3a«beta»,3b«beta»,4«beta»,5«beta»,6a«beta»,7«alpha»,7a«beta»,8R*)- SD 2614 «delta»-Keto 153
Inchi:	InChI=1S/C12H8Cl6O/c13-8-9(14)6-2-1-3(7(6)19)4-5(2)11(9,16)12(17,18)10(4,8)15/h2-6
InchiKey:	IHZHFAQWVKBTSL-UHFFFAOYSA-N
Formula:	C12H8Cl6O
SMILES:	O=C1C2CC3C1C1(Cl)C(Cl)C4(Cl)C2C3C1(Cl)C4(Cl)Cl
Mol. weight [g/mol]:	380.91
CAS:	53494-70-5

Physical Properties

Property code	Value	Unit	Source
gf	135.53	kJ/mol	Joback Method
hf	-181.41	kJ/mol	Joback Method
hfus	28.67	kJ/mol	Joback Method
hvap	65.76	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.809		Crippen Method
mcvol	200.650	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
tb	764.86	K	Joback Method
tc	1044.80	K	Joback Method
tf	647.40	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.22	J/molxK	764.86	Joback Method
cpg	542.35	J/molxK	811.52	Joback Method
cpg	560.92	J/molxK	858.17	Joback Method
cpg	582.98	J/molxK	904.83	Joback Method
cpg	609.57	J/molxK	951.48	Joback Method

cpg	641.73	J/mol×K	998.14	Joback Method
cpg	680.50	J/mol×K	1044.80	Joback Method

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=C53494705&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	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

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