

1,4:5,8-Dimethanonaphthalen-2-ol, 3,5,6,7,8,9,9-heptachloro-1,2,3,4,4a,5,8,8a-octahydro- (1«alpha»,2«alpha»,3«beta»,4«alpha»,4a«beta»,5«alpha»,6«beta»,7«beta»,8«beta»,9«beta»)heptachloro-1,2,3,4,4a,5,8,8a-octahydro-1,4:5,8-dimethanonaphthalen-2-ol

Other names: Dieldrin, chlorhydrin
Inchi: InChI=1S/C12H9Cl7O/c13-6-2-1-3(7(6)20)5-4(2)10(16)8(14)9(15)11(5,17)12(10,18)19/h2
InchiKey: KAKBPXOZYDVIGI-UHFFFAOYSA-N
Formula: C12H9Cl7O
SMILES: OC1C(Cl)C2CC1C1C2C2(Cl)C(Cl)=C(Cl)C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]: 417.37
CAS: 62059-42-1

Physical Properties

Property code	Value	Unit	Source
gf	28.51	kJ/mol	Joback Method
hf	-283.36	kJ/mol	Joback Method
hfus	39.75	kJ/mol	Joback Method
hvap	85.95	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.682		Crippen Method
mcvol	223.750	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
tb	841.60	K	Joback Method
tc	1089.46	K	Joback Method
tf	643.32	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.83	J/molxK	841.60	Joback Method
cpg	592.96	J/molxK	882.91	Joback Method
cpg	611.17	J/molxK	924.22	Joback Method
cpg	632.02	J/molxK	965.53	Joback Method
cpg	656.06	J/molxK	1006.84	Joback Method
cpg	683.85	J/molxK	1048.15	Joback Method
cpg	715.93	J/molxK	1089.46	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=C62059421&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
hvp:	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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