

«alpha»-Chlordene

Other names:	1,4-Ethenopentalene, 1,2,3,5,7,8-hexachloro-1,3a,4,5,6,6a-hexahydro-, (1«alpha»,3a«alpha»,4«beta»,5«alpha»,6a«alpha»)-
Inchi:	InChI=1S/C10H6Cl6/c11-3-1-2-4-5(3)7(13)9(15)10(2,16)8(14)6(4)12/h2-5H,1H2
InchiKey:	GSNLXLNDMLYEEK-UHFFFAOYSA-N
Formula:	C10H6Cl6
SMILES:	C1C1=C(Cl)C2(Cl)C(Cl)=C(Cl)C3C1C(Cl)CC32
Mol. weight [g/mol]:	338.87
CAS:	56534-02-2

Physical Properties

Property code	Value	Unit	Source
gf	132.38	kJ/mol	Joback Method
hf	-87.69	kJ/mol	Joback Method
hfus	35.88	kJ/mol	Joback Method
hvap	65.54	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.229		Crippen Method
mcvol	184.020	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1854.00		NIST Webbook
tb	686.41	K	Joback Method
tc	943.87	K	Joback Method
tf	499.30	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.62	J/molxK	686.41	Joback Method
cpg	405.84	J/molxK	729.32	Joback Method
cpg	415.64	J/molxK	772.23	Joback Method
cpg	425.29	J/molxK	815.14	Joback Method
cpg	435.06	J/molxK	858.05	Joback Method
cpg	445.23	J/molxK	900.96	Joback Method
cpg	456.08	J/molxK	943.87	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=C56534022&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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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