

2,5-Methano-2H-indeno[1,2-b]oxirene, 2,3,4,5,6,6a,7,7-octachloro-1a,1b,5,5a,6,6a-hexahydro- (1a«alpha»,1b«beta»,2«alpha»,5«alpha»,5a«beta»

Other names: 1,7-Methanoindan, 1,2,3,5,6,7,8-octachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-
ex, 2,3,4,5,6,6a,7,7-octachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-
4,7-Methanoindan, 1,2,4,5,6,7,8,8-octachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-

Octachlor epoxide

Oxychlordan

Oxychlordane

Inchi: 2,3,4,5,6,6A,7,7-octachloro-1a,1b,5,5a,6,6a-hexahydro-2,5-methano-2H-indeno-[1,2-b]oxirene (oxychlordan)
InchiKey: VWGNQYSIWFHEQU-UHFFFAOYSA-N
Formula: C10H4Cl8O
SMILES: ClC1=C(Cl)C2(Cl)C3C4OC4(Cl)C(Cl)C3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]: 423.76
CAS: 27304-13-8

Physical Properties

Property code	Value	Unit	Source
gf	64.76	kJ/mol	Joback Method
hf	-195.85	kJ/mol	Joback Method
hfus	37.39	kJ/mol	Joback Method
hvap	72.70	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.019		Crippen Method
mcvol	207.810	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1982.00		NIST Webbook
rinpol	2071.00		NIST Webbook
tb	768.68	K	Joback Method
tc	1052.88	K	Joback Method
tf	648.11	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.48	J/molxK	1005.51	Joback Method

cpg	460.71	J/mol×K	768.68	Joback Method
cpg	472.87	J/mol×K	816.05	Joback Method
cpg	487.89	J/mol×K	863.41	Joback Method
cpg	506.81	J/mol×K	910.78	Joback Method
cpg	530.66	J/mol×K	958.14	Joback Method
cpg	597.32	J/mol×K	1052.88	Joback Method
hvapt	75.00	kJ/mol	388.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27304138&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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