

Chlordene epoxide

Other names:	Chlordene epoxide 2,5-Methano-2H-indeno(1,2-b)oxirene, 2,3,4,5,7,7-hexachloro-1a,1b,5,5a,6,6a-hexahydro- 3a,4,7,7a-Tetrahydro-1,2-epoxy-4,5,6,7,8,8-hexachloro-4,7-methanoindan
Inchi:	InChI=1S/C10H6Cl6O/c11-6-7(12)9(14)4-2(1-3-5(4)17-3)8(6,13)10(9,15)16/h2-5H,1H2
InchiKey:	VMNNMBZKONGDDQ-UHFFFAOYSA-N
Formula:	C10H6Cl6O
SMILES:	C1C1=C(Cl)C2(Cl)C3C4OC4CC3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]:	354.87

Physical Properties

Property code	Value	Unit	Source
hfus	34.22	kJ/mol	Joback Method
log10ws	-5.82		Cheméo Relay (1.0)
logp	4.235		Crippen Method
mcvol	183.330	ml/mol	McGowan Method
tf	402.21	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.70	J/mol×K	698.25	Joback Method
cpg	433.89	J/mol×K	743.31	Joback Method
cpg	444.73	J/mol×K	788.36	Joback Method
cpg	456.93	J/mol×K	833.42	Joback Method
cpg	471.25	J/mol×K	878.48	Joback Method
cpg	488.41	J/mol×K	923.53	Joback Method
cpg	509.16	J/mol×K	968.59	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6058237&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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