«alpha»-Chlorodene

Inchi: InChI=1S/C10H6Cl6/c11-6-7(12)9(14)5-3-1-2-4(5)8(6,13)10(9,15)16/h1-2,4-5H,3H2
InchiKey: XCJXQCUJXDUNDN-UHFFFAOYSA-N
Formula: C10H6Cl6
SMILES: ClC1=C(Cl)C2(Cl)C3CC=CC3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]: 338.87

Physical Properties

Property code	Value	Unit	Source
hfus	24.06	kJ/mol	Joback Method
log10ws	-6.00		Cheméo Relay (1.0)
logp	5.024		Crippen Method
mcvol	184.020	ml/mol	McGowan Method
rinpol	1854.00		NIST Webbook
tf	341.49	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.21	J/mol×K	676.93	Joback Method
cpg	401.11	J/mol×K	723.11	Joback Method
cpg	411.33	J/mol×K	769.30	Joback Method
cpg	422.59	J/mol×K	815.48	Joback Method
cpg	435.62	J/mol×K	861.66	Joback Method
cpg	451.15	J/mol×K	907.84	Joback Method
cpg	469.90	J/mol×K	954.03	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R595227&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/ci990307l
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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point