«beta»-Dihydroheptachlor

Other names: Dihydroheptachlor
Inchi: InChI=1S/C10H7Cl7/c11-4-2-1-3-5(4)9(15)7(13)6(12)8(3,14)10(9,16)17/h3-5H,1-2H2
InchiKey: DRKYTUDHOKREMS-UHFFFAOYSA-N
Formula: C10H7Cl7
SMILES: ClC1=C(Cl)C2(Cl)C3C(Cl)CCC3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]: 375.33
CAS: 14168-01-5

Physical Properties

Property code	Value	Unit	Source
gf	91.06	kJ/mol	Joback Method
hf	-128.13	kJ/mol	Joback Method
hfus	28.10	kJ/mol	Joback Method
hvap	65.70	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.465		Crippen Method
mcvol	200.560	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	2006.60		NIST Webbook
rinpol	2025.90		NIST Webbook
rinpol	2029.80		NIST Webbook
rinpol	1973.50		NIST Webbook
rinpol	1993.40		NIST Webbook
rinpol	2017.90		NIST Webbook
rinpol	2029.00		NIST Webbook
rinpol	2037.90		NIST Webbook
rinpol	1998.50		NIST Webbook
rinpol	1956.80		NIST Webbook
rinpol	1998.50		NIST Webbook
rinpol	2018.70		NIST Webbook
rinpol	2044.70		NIST Webbook
rinpol	1956.80		NIST Webbook
rinpol	1991.90		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1968.20		NIST Webbook
rinpol	1973.50		NIST Webbook
rinpol	1972.70		NIST Webbook

rinpol	2044.70		NIST Webbook
tb	710.53	K	Joback Method
tc	986.90	K	Joback Method
tf	546.98	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.11	J/mol×K	710.53	Joback Method
cpg	449.58	J/mol×K	756.59	Joback Method
cpg	461.75	J/mol×K	802.65	Joback Method
cpg	475.35	J/mol×K	848.72	Joback Method
cpg	491.07	J/mol×K	894.78	Joback Method
cpg	509.61	J/mol×K	940.84	Joback Method
cpg	531.69	J/mol×K	986.90	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C14168015&Units=SI

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: 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