Ethane, hexachloro-

Other names:	1,1,1,2,2,2-Hexachloroethane
	AVLOTHANE
	C2Cl6
	CARBON HEXACHLORIDE
	CCl3CCl3
	Distokal
	Distopan
	Distopin
	Egitol
	Ethane hexachloride
	Ethane, 1,1,1,2,2,2-hexachloro-
	Ethylene hexachloride
	Falkitol
	Fasciolin
	Fron 110
	Hexachlor-aethan
	Hexachlorethane
	Hexachloroethane
	Hexachloroethylene
	Mottenhexe
	NA 9037
	NCI-C04604
	NSC 9224
	PERCHLOROETHANE
	Phenohep
	Rcra waste number U131
Inchi:	InChI=1S/C2Cl6/c3-1(4,5)2(6,7)8
InchiKey:	VHHHONWQHHHLTI-UHFFFAOYSA-N
Formula:	C2Cl6
SMILES:	ClC(Cl)(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	236.74
CAS:	67-72-1

Physical Properties

Property code	Value	Unit	Source
af	0.2750		KDB

chs	-727.00 ± 8.00	kJ/mol	NIST Webbook
ea	1.48 ± 0.10	eV	NIST Webbook
gf	-99.94	kJ/mol	Joback Method
hf	-148.20 ± 5.70	kJ/mol	NIST Webbook
hf	-143.50 ± 9.40	kJ/mol	NIST Webbook
hfl	-199.20 ± 6.10	kJ/mol	NIST Webbook
hfus	11.29	kJ/mol	Joback Method
hsub	59.00 ± 0.80	kJ/mol	NIST Webbook
hvap	51.00 ± 2.30	kJ/mol	NIST Webbook
ie	11.10	eV	NIST Webbook
ie	11.22	eV	NIST Webbook
ie	11.22	eV	NIST Webbook
log10ws	-3.67		Estimated Solubility Method
log10ws	-3.67		Aqueous Solubility Prediction Method
logp	3.727		Crippen Method
mcvol	112.480	ml/mol	McGowan Method
pc	3940.00	kPa	KDB
rinpol	1058.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	176.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1057.80		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1068.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1444.17		NIST Webbook
ripol	1444.17		NIST Webbook
ripol	1461.57		NIST Webbook
ripol	1426.53		NIST Webbook
ss	237.30	J/mol×K	NIST Webbook

tb	458.00 ± 1.00	K	NIST Webbook
tb	459.20	K	KDB
tb	458.00 ± 1.00	K	NIST Webbook
tc	704.40	K	KDB
tf	458.00	K	KDB
tf	461.98	K	Aqueous Solubility Prediction Method
vc	0.419	m3/kmol	KDB
zc	0.2822100		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.23	J/mol×K	710.67	Joback Method
cpg	161.53	J/mol×K	504.51	Joback Method
cpg	164.90	J/mol×K	545.74	Joback Method
cpg	167.57	J/mol×K	586.98	Joback Method
cpg	169.62	J/mol×K	628.21	Joback Method
cpg	171.14	J/mol×K	669.44	Joback Method
cpg	157.38	J/mol×K	463.28	Joback Method
cps	218.00	J/mol×K	298.50	NIST Webbook
cps	198.24	J/mol×K	298.15	NIST Webbook
dvisc	0.0053154	Pa×s	296.66	Joback Method
dvisc	0.0012053	Pa×s	379.97	Joback Method
dvisc	0.0018282	Pa×s	352.20	Joback Method
dvisc	0.0008410	Pa×s	407.74	Joback Method
dvisc	0.0006144	Pa×s	435.51	Joback Method
dvisc	0.0004660	Pa×s	463.28	Joback Method
dvisc	0.0029781	Pa×s	324.43	Joback Method
hfust	9.75	kJ/mol	458.00	NIST Webbook
hfust	2.57	kJ/mol	318.00	NIST Webbook
hfust	9.75	kJ/mol	458.00	NIST Webbook
hfust	8.22	kJ/mol	345.00	NIST Webbook
hsubt	58.90	kJ/mol	331.00	NIST Webbook
hsubt	50.50	kJ/mol	394.00	NIST Webbook
hsubt	59.00	kJ/mol	310.50	NIST Webbook
hvapt	51.20	kJ/mol	402.50	NIST Webbook
hvapt	53.70	kJ/mol	381.50	NIST Webbook
hvapt	40.30	kJ/mol	486.50	NIST Webbook
hvapt	49.00	kJ/mol	459.20	KDB
sfust	23.83	J/mol×K	345.00	NIST Webbook

sfust	8.07	J/mol×K	318.00	NIST Webbook
sfust	21.29	J/mol×K	458.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30211e+01
Coeff. B	-2.79600e+03
Coeff. C	-1.25251e+02
Temperature range (K), min.	344.83
Temperature range (K), max.	487.92

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.45610e+01
Coeff. B	-9.86248e+03
Coeff. C	-1.12902e+01
Coeff. D	3.12000e-06
Temperature range (K), min.	306.15
Temperature range (K), max.	698.00

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C67721&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Influence of Temperature and Surfactants on the Solubilization of Hexachlorobutadiene and Hexachloroethane: https://www.doi.org/10.1021/acs.jced.7b00320

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1544

KDB: https://www.cheric.org/files/research/kdb/mol/mol1544.mol

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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