1,3-Butadiene, 1,1,2,3,4,4-hexachloro-

Other names: 1,1,2,3,4,4-Hexachloro-1,3-butadiene
1,1,2,3,4,4-Hexachloro-buta-1,3-diene
1,1,2,3,4,4-hexachlorobuta-1,3-diene
1,3-Butadiene, hexachloro-
1,3-Hexachlorobutadiene
Butadiene, hexachloro-
C 46
Dolen-pur
Gp-40-66:120
HCB
HCBD
Hexachlor-1,3-butadien
Hexachlorbutadiene
Hexachloro-1,3-Butadiene
Hexachlorobutadiene
Hexachlorobutadiene-(1,3)
NSC 3701
PERCHLOROBUTADIENE
Perchloro-1,3-butadiene
Rcra waste number U128
UN 2279
hexachlorobuta-1,3-diene

Inchi: InChI=1S/C4Cl6/c5-1(3(7)8)2(6)4(9)10

InchiKey: RWNKSTSCBHKHTB-UHFFFAOYSA-N

Formula: C4Cl6

SMILES: ClC(Cl)=C(Cl)C(Cl)=C(Cl)Cl

Mol. weight [g/mol]: 260.76

CAS: 87-68-3

Physical Properties

Property code	Value	Unit	Source
chl	-1691.70 ± 3.30	kJ/mol	NIST Webbook
gf	37.46	kJ/mol	Joback Method
hf	-25.05	kJ/mol	Joback Method
hfl	-24.50 ± 3.60	kJ/mol	NIST Webbook
hfus	26.46	kJ/mol	Joback Method

hvap	51.04	kJ/mol	Joback Method
log10ws	-4.91		Aqueous Solubility Prediction Method
log10ws	-4.92		Estimated Solubility Method
logp	4.757		Crippen Method
mcvol	132.060	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	1206.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	205.80		NIST Webbook
rinpol	1233.94		NIST Webbook
rinpol	205.80		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1229.98		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1231.20		NIST Webbook
rinpol	1231.20		NIST Webbook
rinpol	1196.10		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1480.00		NIST Webbook
tb	488.20	K	NIST Webbook
tc	772.00	K	Joback Method
tf	248.36	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.20	J/mol×K	689.11	Joback Method
cpg	200.49	J/mol×K	730.56	Joback Method
cpg	184.96	J/mol×K	523.34	Joback Method
cpg	189.05	J/mol×K	564.78	Joback Method
cpg	192.56	J/mol×K	606.23	Joback Method
cpg	195.59	J/mol×K	647.67	Joback Method
cpg	202.54	J/mol×K	772.00	Joback Method
hvapt	58.60	kJ/mol	413.50	NIST Webbook
hvapt	60.40	kJ/mol	408.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.26620e+01
Coeff. B	-2.95853e+03
Coeff. C	-1.20391e+02
Temperature range (K), min.	359.48
Temperature range (K), max.	522.88

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.63392e+01
Coeff. B	-8.06986e+03
Coeff. C	-3.97881e+00
Coeff. D	-2.27853e-06
Temperature range (K), min.	252.15
Temperature range (K), max.	741.00

Sources

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1742.mol

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1742

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

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

Determination of Henry's Law Constants Using Internal Standards and Purge and Trap Gas Chromatography: https://www.doi.org/10.1021/je3010535

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C87683&Units=SI

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

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

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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume