

Benzene, hexachloro-

Other names:	1,2,3,4,5,6-Hexachlorobenzene AMATIN ANTICARIE Benzene, 1,2,3,4,5,6-hexachloro- Bunt-cure Bunt-no-more Ceku C.B. Co-op Hexa Esachlorobenzene Granox nm HCB Hexa C.B. Hexachlorbenzol Hexachlorobenzene Hexcachlorbenzen Julin's carbon chloride Julin's chloride NSC 9243 No Bunt No Bunt 40 No Bunt 80 No Bunt Liquid PENTACHLOROPHENYLCHLORIDE Pentachlorophenyl chloride Perchlorobenzene Phenyl perchloryl Rcra waste number U127 Saatbeizfungizid Sanocid Sanocide Smut-Go Snieciotox UN 2729
Inchi:	InChI=1S/C6Cl6/c7-1-2(8)4(10)6(12)5(11)3(1)9
InchiKey:	CKAPSXZOOQJIBF-UHFFFAOYSA-N
Formula:	C6Cl6
SMILES:	Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	284.78
CAS:	118-74-1

Physical Properties

Property code	Value	Unit	Source
af	0.5430		KDB
chs	-2375.30 ± 4.20	kJ/mol	NIST Webbook
chs	-2361.09	kJ/mol	NIST Webbook
ea	0.92 ± 0.10	eV	NIST Webbook
ea	1.00	eV	NIST Webbook
gf	-7.68	kJ/mol	Joback Method
hf	-44.70	kJ/mol	NIST Webbook
hfs	-141.77	kJ/mol	NIST Webbook
hfs	-127.60 ± 4.20	kJ/mol	NIST Webbook
hfus	23.92	kJ/mol	Johari-Goldstein relaxation in orientationally disordered phase of hexa-substituted benzenes
hsub	96.80 ± 0.50	kJ/mol	NIST Webbook
hsub	90.50 ± 0.20	kJ/mol	NIST Webbook
hvap	74.40 ± 0.70	kJ/mol	NIST Webbook
hvap	76.80	kJ/mol	NIST Webbook
ie	8.98	eV	NIST Webbook
ie	9.00 ± 0.10	eV	NIST Webbook
ie	9.19 ± 0.03	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
ie	9.31 ± 0.05	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-7.62		Aqueous Solubility Prediction Method
logp	5.607		Crippen Method
mcvol	145.080	ml/mol	McGowan Method
pc	3230.00	kPa	KDB
rinpol	1691.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1724.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1690.00		NIST Webbook

rinpol	1691.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1739.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1734.00		NIST Webbook
rinpol	1734.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	291.00		NIST Webbook
rinpol	289.80		NIST Webbook
rinpol	288.81		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1734.00		NIST Webbook
rinpol	1700.10		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	287.10		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1678.00		NIST Webbook
ripol	2153.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2202.30		NIST Webbook
ripol	2178.00		NIST Webbook
ripol	2153.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2204.00		NIST Webbook
ss	260.24	J/mol×K	NIST Webbook
tb	582.60	K	KDB
tb	597.70	K	NIST Webbook
tc	825.80	K	KDB
tf	505.00 ± 0.10	K	NIST Webbook
tf	500.00 ± 2.50	K	NIST Webbook
tf	501.10 ± 0.20	K	NIST Webbook
tf	501.27 ± 0.20	K	NIST Webbook

tf	503.12	K	Aqueous Solubility Prediction Method
tf	503.00	K	KDB
tf	502.80 ± 0.50	K	NIST Webbook
tt	502.02 ± 0.01	K	NIST Webbook
vc	0.557	m3/kmol	KDB
zc	0.2622620		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.03	J/mol×K	783.43	Joback Method
cpg	237.95	J/mol×K	868.72	Joback Method
cpg	228.60	J/mol×K	740.78	Joback Method
cpg	224.86	J/mol×K	698.13	Joback Method
cpg	220.80	J/mol×K	655.49	Joback Method
cpg	216.40	J/mol×K	612.84	Joback Method
cpg	235.14	J/mol×K	826.07	Joback Method
cps	201.29	J/mol×K	298.15	NIST Webbook
cps	257.70	J/mol×K	299.80	NIST Webbook
dvisc	0.0003671	Pa×s	550.53	Joback Method
dvisc	0.0004409	Pa×s	519.38	Joback Method
dvisc	0.0005419	Pa×s	488.23	Joback Method
dvisc	0.0006852	Pa×s	457.07	Joback Method
dvisc	0.0002692	Pa×s	612.84	Joback Method
dvisc	0.0008967	Pa×s	425.92	Joback Method
dvisc	0.0003117	Pa×s	581.69	Joback Method
hfust	25.20	kJ/mol	502.00	NIST Webbook
hfust	23.85	kJ/mol	505.00	NIST Webbook
hfust	23.85	kJ/mol	505.00	NIST Webbook
hfust	25.18	kJ/mol	502.02	NIST Webbook
hfust	24.96	kJ/mol	501.87	NIST Webbook
hsubt	92.00 ± 8.20	kJ/mol	383.00	NIST Webbook
hsubt	79.50 ± 1.20	kJ/mol	324.50	NIST Webbook
hsubt	101.30	kJ/mol	303.00	NIST Webbook
hsubt	62.70	kJ/mol	444.50	NIST Webbook
hsubt	85.50	kJ/mol	483.50	NIST Webbook
hsubt	105.00	kJ/mol	285.50	NIST Webbook
hsubt	89.60 ± 0.20	kJ/mol	337.00	NIST Webbook
hsubt	94.70	kJ/mol	343.50	NIST Webbook
hsubt	77.40 ± 0.80	kJ/mol	278.00	NIST Webbook

hvapt	68.70	kJ/mol	545.50	NIST Webbook
hvapt	68.60	kJ/mol	398.00	NIST Webbook
hvapt	81.30	kJ/mol	285.50	NIST Webbook
hvapt	63.59	kJ/mol	582.60	KDB
hvapt	60.50	kJ/mol	484.50	NIST Webbook
psub	0.07	kPa	411.90	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.05	kPa	405.30	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.06	kPa	405.80	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.05	kPa	406.10	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.06	kPa	406.50	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.06	kPa	407.00	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit

psub	0.06	kPa	407.40	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.06	kPa	407.80	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.07	kPa	408.20	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.07	kPa	408.60	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.08	kPa	409.00	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.07	kPa	409.40	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.08	kPa	409.80	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit

psub	0.08	kPa	410.20	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
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psub	0.09	kPa	411.40	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.06	kPa	404.90	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.08	kPa	412.30	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.08	kPa	412.70	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit

psub	0.08	kPa	413.20	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.09	kPa	413.60	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
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psub	0.09	kPa	414.40	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
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psub	0.10	kPa	415.70	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit

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psub	0.16	kPa	423.20	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.15	kPa	423.60	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.15	kPa	424.00	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.15	kPa	424.40	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit

psub	0.17	kPa	424.80	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.17	kPa	425.70	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	1.44e-03	kPa	358.00	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	2.16e-03	kPa	362.90	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	3.73e-03	kPa	368.90	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	5.19e-03	kPa	373.10	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions

psub	7.71e-03	kPa	377.80	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.01	kPa	382.90	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.05	kPa	404.50	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.02	kPa	392.80	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.03	kPa	397.90	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.05	kPa	402.80	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions

psub	0.06	kPa	404.10	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.05	kPa	403.60	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.06	kPa	402.80	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.05	kPa	402.00	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.05	kPa	401.20	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.04	kPa	400.80	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.05	kPa	400.40	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit

psub	0.04	kPa	397.50	Vapor Pressures and Standard Molar Enthalpies, Entropies and Gibbs energies of Sublimation of two hexachloro herbicides using a TG unit
psub	0.02	kPa	389.00	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
sfust	50.20	J/mol×K	502.02	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.18922e+01
Coeff. B	-2.91145e+03
Coeff. C	-1.97439e+02
Temperature range (K), min.	448.33
Temperature range (K), max.	639.86

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	-1.10122e+02
Coeff. B	-1.18239e+03
Coeff. C	1.89428e+01
Coeff. D	-1.14651e-05
Temperature range (K), min.	387.15
Temperature range (K), max.	825.00

Sources

The Yaws Handbook of Vapor

Pressure:

KDB Vapor Pressure Data:

KDB:

Crippen Method:

Vapor Pressures and Standard Molar

Enthalpies, Entropies and Gibbs

Free Energies of Formation and

Heat Capacities of Organic Compounds

in the Gaseous State: Aqueous Unit:

Standard Enthalpies of Formation of

Selected Chlorobenzenes:

and Chlorophenols: Ambient

Temperature and Henry's Law Constant

for Diffusion in Air and Water:

Boundary Layers:

Joback Method:

Aqueous Solubility Prediction Method:

Johari-Goldstein relaxation in

orientationally disordered phase of

hexa-substituted benzenes:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1664>

<https://www.thermo.com/files/research/kdb/mol/mol1664.mol>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

<https://www.doi.org/10.1016/j.tca.2009.10.017>

<https://www.doi.org/10.1021/je034170d>

<https://www.doi.org/10.1021/je060429r>

<https://www.doi.org/10.1021/je300954s>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C118741&Units=SI>

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

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

<https://www.doi.org/10.1016/j.tca.2015.01.017>

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

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
hfs:	Solid 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
psub:	Sublimation 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
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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