

«alpha»-Lindane

Other names:	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1«alpha»,2«alpha»,3«beta»,4«alpha»,5«beta»,6«beta»)- Cyclohexane, 1,2,3,4,5,6-hexachloro-, «alpha»- «alpha»-Benzene hexachloride «alpha»-Hexachloran «alpha»-Hexachlorane «alpha»-Hexachlorcyclohexane «alpha»-Hexachlorocyclohexane «alpha»-HCH «alpha»-1,2,3,4,5,6-Hexachlorcyclohexane «alpha»-1,2,3,4,5,6-Hexachlorocyclohexane Cyclohexane, 1,2,3,4,5,6-hexachloro-, «alpha»-isomer Benzene hexachloride-«alpha»-isomer Cyclohexane, «alpha»-1,2,3,4,5,6-hexachloro- ENT 9,232 Hexachlorcyclohexan 1-«alpha»,2-«alpha»,3-«beta»,4-«alpha»,5-«beta»,6-«beta»-Hexachlorocyclohexane BHC-«alpha» isomer BHC «alpha» «alpha»-BHC HCH-«alpha» (.+/.)-«alpha»-Hexachlorocyclohexane 1a,2a,3b,4a,5b,6b-Hexachlorocyclohexane Benzene hexachloride-alpha-isomer 1,2,3,4,5,6-Hexachlorocyclohexane, (1«alpha»,2«alpha»,3«beta»,4«alpha»,5«beta»,6«beta»)-1,2,3,4,5,6-hexachlorocyclohexane
Inchi:	InChI=1S/C6H6Cl6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-6H/t1-,2-,3-,4-,5+,6+/m1/s1
InchiKey:	JLYXXMFPNIAWKQ-SHFUYGGZSA-N
Formula:	C6H6Cl6
SMILES:	C1C1C(CI)C(CI)C(CI)C(CI)C1Cl
Mol. weight [g/mol]:	290.83
CAS:	319-84-6

Physical Properties

Property code	Value	Unit	Source
chs	-2959.60 ± 2.20	kJ/mol	NIST Webbook
chs	-2742.40 ± 0.80	kJ/mol	NIST Webbook

gf	-86.04		kJ/mol	Joback Method
hf	-308.99		kJ/mol	Joback Method
hfs	-172.50		kJ/mol	NIST Webbook
hfs	-400.80 ± 2.50		kJ/mol	NIST Webbook
hfus	33.67		kJ/mol	Joback Method
hvap	54.14		kJ/mol	Joback Method
log10ws	-3.82			Crippen Method
logp	3.644			Crippen Method
mcvol	157.980		ml/mol	McGowan Method
pc	2561.10		kPa	Joback Method
rinpol	1640.00			NIST Webbook
rinpol	1645.00			NIST Webbook
rinpol	1681.00			NIST Webbook
rinpol	1690.00			NIST Webbook
rinpol	1655.00			NIST Webbook
rinpol	1657.00			NIST Webbook
rinpol	1690.00			NIST Webbook
rinpol	1659.00			NIST Webbook
rinpol	289.00			NIST Webbook
rinpol	1656.00			NIST Webbook
rinpol	1657.00			NIST Webbook
rinpol	1659.00			NIST Webbook
rinpol	1724.00			NIST Webbook
rinpol	1714.00			NIST Webbook
rinpol	1645.00			NIST Webbook
rinpol	1655.00			NIST Webbook
rinpol	1657.00			NIST Webbook
ripol	2452.00			NIST Webbook
ripol	2452.00			NIST Webbook
tb	557.46		K	Joback Method
tc	799.93		K	Joback Method
tf	431.20 ± 0.70		K	NIST Webbook
tf	429.00 ± 4.00		K	NIST Webbook
tf	430.50 ± 0.20		K	NIST Webbook
vc	0.594		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.54	J/mol×K	557.46	Joback Method
cpg	314.57	J/mol×K	597.87	Joback Method

cpg	326.75	J/mol×K	638.28	Joback Method
cpg	338.08	J/mol×K	678.70	Joback Method
cpg	348.54	J/mol×K	719.11	Joback Method
cpg	358.13	J/mol×K	759.52	Joback Method
cpg	366.85	J/mol×K	799.93	Joback Method
dvisc	0.0011967	Paxs	362.14	Joback Method
dvisc	0.0015575	Paxs	323.08	Joback Method
dvisc	0.0009679	Paxs	401.21	Joback Method
dvisc	0.0008129	Paxs	440.27	Joback Method
dvisc	0.0007025	Paxs	479.33	Joback Method
dvisc	0.0006205	Paxs	518.40	Joback Method
dvisc	0.0005577	Paxs	557.46	Joback Method
hsubt	95.70	kJ/mol	338.00	NIST Webbook
hsubt	92.90	kJ/mol	334.00	NIST Webbook
hvapt	68.50	kJ/mol	398.00	NIST Webbook

Sources

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=C319846&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hsubt:	Enthalpy of sublimation at a given temperature
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
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

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