

# Hexane, 1,2-dichloro-

<b>Other names:</b>	(dl) 1,2-dichlorohexane 1,2-Dichlorohexane
<b>Inchi:</b>	InChI=1S/C6H12Cl2/c1-2-3-4-6(8)5-7/h6H,2-5H2,1H3
<b>InchiKey:</b>	ZHFXSKJYCSWRJA-UHFFFAOYSA-N
<b>Formula:</b>	C6H12Cl2
<b>SMILES:</b>	CCCCC(Cl)CCl
<b>Mol. weight [g/mol]:</b>	155.06
<b>CAS:</b>	2162-92-7

## Physical Properties

Property code	Value	Unit	Source
gf	-26.66	kJ/mol	Joback Method
hf	-203.93	kJ/mol	Joback Method
hfus	16.17	kJ/mol	Joback Method
hvap	48.80	kJ/mol	NIST Webbook
hvap	47.90 ± 0.70	kJ/mol	NIST Webbook
hvap	48.16	kJ/mol	NIST Webbook
log10ws	-2.75		Crippen Method
logp	3.023		Crippen Method
mcvol	119.880	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1005.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	980.00		NIST Webbook
ripol	1311.00		NIST Webbook
tb	411.10	K	Joback Method
tc	595.37	K	Joback Method
tf	202.22	K	Joback Method
vc	0.464	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.32	J/mol×K	595.37	Joback Method
cpg	212.27	J/mol×K	411.10	Joback Method
cpg	222.72	J/mol×K	441.81	Joback Method
cpg	232.70	J/mol×K	472.52	Joback Method
cpg	242.24	J/mol×K	503.23	Joback Method
cpg	251.35	J/mol×K	533.95	Joback Method
cpg	260.04	J/mol×K	564.66	Joback Method
dvisc	0.0003162	Paxs	411.10	Joback Method
dvisc	0.0074186	Paxs	202.22	Joback Method
dvisc	0.0029798	Paxs	237.03	Joback Method
dvisc	0.0015119	Paxs	271.85	Joback Method
dvisc	0.0008949	Paxs	306.66	Joback Method
dvisc	0.0005894	Paxs	341.47	Joback Method
dvisc	0.0004194	Paxs	376.29	Joback Method
hvapt	44.90	kJ/mol	397.00	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58942e+01
Coeff. B	-4.31898e+03
Coeff. C	-6.51800e+01
Temperature range (K), min.	341.92
Temperature range (K), max.	473.30

## Sources

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2162927&Units=SI>

**The Yaws Handbook of Vapor**

**Pressure:**

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

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

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

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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