

# 1-Chloro-6-phenylhexane

<b>Inchi:</b>	InChI=1S/C12H17Cl/c13-11-7-2-1-4-8-12-9-5-3-6-10-12/h3,5-6,9-10H,1-2,4,7-8,11H2
<b>InchiKey:</b>	RCVNHNOEUMFFDY-UHFFFAOYSA-N
<b>Formula:</b>	C12H17Cl
<b>SMILES:</b>	C1CCCCC1c1ccccc1
<b>Mol. weight [g/mol]:</b>	196.72
<b>CAS:</b>	71434-68-9

## Physical Properties

Property code	Value	Unit	Source
gf	150.64	kJ/mol	Joback Method
hf	-70.22	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	48.97	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	4.028		Crippen Method
mvol	168.420	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	538.07	K	Joback Method
tc	742.35	K	Joback Method
tf	281.34	K	Joback Method
vc	0.648	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.44	J/molxK	538.07	Joback Method
cpg	392.44	J/molxK	572.12	Joback Method
cpg	407.51	J/molxK	606.16	Joback Method
cpg	421.71	J/molxK	640.21	Joback Method
cpg	435.07	J/molxK	674.26	Joback Method
cpg	447.63	J/molxK	708.31	Joback Method
cpg	459.43	J/molxK	742.35	Joback Method
dvisc	0.0034175	Paxs	281.34	Joback Method
dvisc	0.0015793	Paxs	324.13	Joback Method

dvisc	0.0008738	Paxs	366.92	Joback Method
dvisc	0.0005471	Paxs	409.70	Joback Method
dvisc	0.0003743	Paxs	452.49	Joback Method
dvisc	0.0002734	Paxs	495.28	Joback Method
dvisc	0.0002099	Paxs	538.07	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C71434689&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C71434689&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## 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>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>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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