

# Pentane, 2-chloro-4-methyl-

<b>Other names:</b>	2-Chloro-4-methylpentane
<b>Inchi:</b>	InChI=1S/C6H13Cl/c1-5(2)4-6(3)7/h5-6H,4H2,1-3H3
<b>InchiKey:</b>	WIMBRKMSNRCNMP-UHFFFAOYSA-N
<b>Formula:</b>	C6H13Cl
<b>SMILES:</b>	CC(C)CC(C)Cl
<b>Mol. weight [g/mol]:</b>	120.62
<b>CAS:</b>	25346-32-1

## Physical Properties

Property code	Value	Unit	Source
gf	-17.17	kJ/mol	Joback Method
hf	-193.47	kJ/mol	Joback Method
hfus	8.45	kJ/mol	Joback Method
hvap	32.56	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.660		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	763.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	800.00		NIST Webbook
tb	373.23	K	Joback Method
tc	553.82	K	Joback Method
tf	157.30	K	Joback Method
vc	0.408	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.75	J/mol×K	373.23	Joback Method
cpg	196.81	J/mol×K	403.33	Joback Method
cpg	207.42	J/mol×K	433.43	Joback Method

cpg	217.60	J/mol×K	463.52	Joback Method
cpg	227.35	J/mol×K	493.62	Joback Method
cpg	236.69	J/mol×K	523.72	Joback Method
cpg	245.63	J/mol×K	553.82	Joback Method
dvisc	0.0170744	Paxs	157.30	Joback Method
dvisc	0.0045226	Paxs	193.29	Joback Method
dvisc	0.0018178	Paxs	229.28	Joback Method
dvisc	0.0009357	Paxs	265.26	Joback Method
dvisc	0.0005644	Paxs	301.25	Joback Method
dvisc	0.0003793	Paxs	337.24	Joback Method
dvisc	0.0002752	Paxs	373.23	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43566e+01
Coeff. B	-3.39655e+03
Coeff. C	-4.85000e+01
Temperature range (K), min.	289.92
Temperature range (K), max.	424.01

## Sources

<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>
<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=C25346321&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25346321&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpolar:</b>	Non-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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