

# Pentane, 3-(chloromethyl)

<b>Other names:</b>	3-(chloromethyl)pentane
<b>Inchi:</b>	InChI=1S/C6H13Cl/c1-3-6(4-2)5-7/h6H,3-5H2,1-2H3
<b>InchiKey:</b>	PQHNRODYYLFLRE-UHFFFAOYSA-N
<b>Formula:</b>	C6H13Cl
<b>SMILES:</b>	CCC(CC)CCI
<b>Mol. weight [g/mol]:</b>	120.62
<b>CAS:</b>	4737-41-1

## Physical Properties

Property code	Value	Unit	Source
gf	-14.73	kJ/mol	Joback Method
hf	-188.19	kJ/mol	Joback Method
hfus	11.97	kJ/mol	Joback Method
hvap	32.95	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.661		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	815.00		NIST Webbook
rinpol	815.00		NIST Webbook
tb	399.15 ± 3.00	K	NIST Webbook
tc	550.01	K	Joback Method
tf	172.30	K	Joback Method
vc	0.414	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.85	J/mol×K	373.67	Joback Method
cpg	235.29	J/mol×K	520.62	Joback Method
cpg	226.20	J/mol×K	491.23	Joback Method
cpg	216.72	J/mol×K	461.84	Joback Method
cpg	206.84	J/mol×K	432.45	Joback Method
cpg	196.56	J/mol×K	403.06	Joback Method

cpg	244.00	J/molxK	550.01	Joback Method
dvisc	0.0002833	Paxs	373.67	Joback Method
dvisc	0.0003773	Paxs	340.11	Joback Method
dvisc	0.0005349	Paxs	306.55	Joback Method
dvisc	0.0008264	Paxs	272.99	Joback Method
dvisc	0.0014423	Paxs	239.42	Joback Method
dvisc	0.0030184	Paxs	205.86	Joback Method
dvisc	0.0084225	Paxs	172.30	Joback Method

## Sources

<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=C4737411&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4737411&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>rinpol:</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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