

# 1-Chloro-4-decyne

<b>Inchi:</b>	InChI=1S/C10H17Cl/c1-2-3-4-5-6-7-8-9-10-11/h2-5,8-10H2,1H3
<b>InchiKey:</b>	WQROTKWHQIGFTO-UHFFFAOYSA-N
<b>Formula:</b>	C10H17Cl
<b>SMILES:</b>	CCCCC#CCCCCl
<b>Mol. weight [g/mol]:</b>	172.69
<b>CAS:</b>	26817-65-2

## Physical Properties

Property code	Value	Unit	Source
gf	224.19	kJ/mol	Joback Method
hf	6.83	kJ/mol	Joback Method
hfus	28.98	kJ/mol	Joback Method
hvap	44.39	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.589		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
tb	474.63	K	Joback Method
tc	665.33	K	Joback Method
tf	338.48	K	Joback Method
vc	0.607	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.30	J/molxK	474.63	Joback Method
cpg	332.29	J/molxK	506.41	Joback Method
cpg	345.66	J/molxK	538.20	Joback Method
cpg	358.44	J/molxK	569.98	Joback Method
cpg	370.64	J/molxK	601.76	Joback Method
cpg	382.29	J/molxK	633.54	Joback Method
cpg	393.40	J/molxK	665.33	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.00 ± 1.00	K	2.00	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C26817652&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C26817652&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>
<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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>hvp:</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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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