

# 2,10-Dodecadiyne

<b>Inchi:</b>	InChI=1S/C12H18/c1-3-5-7-9-11-12-10-8-6-4-2/h7-12H2,1-2H3
<b>InchiKey:</b>	CNMHMGNWEVHOCK-UHFFFAOYSA-N
<b>Formula:</b>	C12H18
<b>SMILES:</b>	CC#CCCCCCCC#CC
<b>Mol. weight [g/mol]:</b>	162.27
<b>CAS:</b>	31699-38-4

## Physical Properties

Property code	Value	Unit	Source
gf	455.76	kJ/mol	Joback Method
hf	253.59	kJ/mol	Joback Method
hfus	33.08	kJ/mol	Joback Method
hvap	46.61	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.374		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
tb	491.96	K	Joback Method
tc	696.84	K	Joback Method
tf	437.20	K	Joback Method
vc	0.631	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.46	J/mol×K	491.96	Joback Method
cpg	361.21	J/mol×K	526.11	Joback Method
cpg	376.24	J/mol×K	560.25	Joback Method
cpg	390.60	J/mol×K	594.40	Joback Method
cpg	404.28	J/mol×K	628.55	Joback Method
cpg	417.33	J/mol×K	662.70	Joback Method
cpg	429.75	J/mol×K	696.84	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.00	K	1.00	NIST Webbook

## 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=C31699384&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C31699384&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>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>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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