

# 4-Tridecen-6-yne, (E)-

<b>Other names:</b>	(4E)-4-Tridecen-6-yne 4E-tridecen-6-yne
<b>Inchi:</b>	InChI=1S/C13H22/c1-3-5-7-9-11-13-12-10-8-6-4-2/h7,9H,3-6,8,10,12H2,1-2H3/b9-7+
<b>InchiKey:</b>	NPZMKXJJWSFOQL-VQHVLOKHSA-N
<b>Formula:</b>	C13H22
<b>SMILES:</b>	CCCC=CC#CCCCCCC
<b>Mol. weight [g/mol]:</b>	178.31
<b>CAS:</b>	74744-43-7

## Physical Properties

Property code	Value	Unit	Source
gf	341.60	kJ/mol	Joback Method
hf	77.87	kJ/mol	Joback Method
hfus	32.75	kJ/mol	Joback Method
hvap	46.64	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.316		Crippen Method
mvol	181.130	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1607.00		NIST Webbook
rinpol	1607.00		NIST Webbook
tb	510.00	K	Joback Method
tc	697.27	K	Joback Method
tf	337.29	K	Joback Method
vc	0.706	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.01	J/mol×K	510.00	Joback Method
cpg	423.87	J/mol×K	541.21	Joback Method
cpg	439.95	J/mol×K	572.42	Joback Method
cpg	455.29	J/mol×K	603.63	Joback Method
cpg	469.91	J/mol×K	634.85	Joback Method

cpg	483.85	J/mol×K	666.06	Joback Method
cpg	497.13	J/mol×K	697.27	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=C74744437&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C74744437&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>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>rinpola:</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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