

# (E)-Ene-yne-dicyclo ether

<b>Inchi:</b>	InChI=1S/C13H12O2/c1-2-3-4-5-7-12-8-10-13(15-12)9-6-11-14-13/h7-8,10H,6,9,11H2,1H
<b>InchiKey:</b>	WTRXKCNFPMTAJV-GHXNOFRVSA-N
<b>Formula:</b>	C13H12O2
<b>SMILES:</b>	CC#CC#CC=C1C=CC2(CCCO2)O1
<b>Mol. weight [g/mol]:</b>	200.23

## Physical Properties

Property code	Value	Unit	Source
gf	454.78	kJ/mol	Joback Method
hf	265.46	kJ/mol	Joback Method
hfus	35.77	kJ/mol	Joback Method
hvap	58.44	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	1.990		Crippen Method
mcvol	158.250	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	1815.00		NIST Webbook
tb	605.74	K	Joback Method
tc	884.24	K	Joback Method
tf	566.19	K	Joback Method
vc	0.588	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.13	J/molxK	605.74	Joback Method
cpg	400.74	J/molxK	652.16	Joback Method
cpg	416.09	J/molxK	698.57	Joback Method
cpg	430.51	J/molxK	744.99	Joback Method
cpg	444.31	J/molxK	791.41	Joback Method
cpg	457.79	J/molxK	837.83	Joback Method
cpg	471.28	J/molxK	884.24	Joback Method

# Sources

<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=R632801&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R632801&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>

# 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>h vap:</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>m cvol:</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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