

# Cyclopropanecarboxylic acid, tridec-2-ynyl ester

Inchi:	InChI=1S/C17H28O2/c1-2-3-4-5-6-7-8-9-10-11-12-15-19-17(18)16-13-14-16/h16H,2-10,17H
InchiKey:	OSELOIIMCUZBT-UHFFFAOYSA-N
Formula:	C17H28O2
SMILES:	CCCCCCCCC#CCOC(=O)C1CC1
Mol. weight [g/mol]:	264.40

## Physical Properties

Property code	Value	Unit	Source
gf	121.89	kJ/mol	Joback Method
hf	-293.91	kJ/mol	Joback Method
hfus	43.83	kJ/mol	Joback Method
hvap	64.66	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.474		Crippen Method
mcvol	238.370	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
tb	680.39	K	Joback Method
tc	870.83	K	Joback Method
tf	477.55	K	Joback Method
vc	0.930	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.13	J/molxK	680.39	Joback Method
cpg	694.39	J/molxK	712.13	Joback Method
cpg	711.73	J/molxK	743.87	Joback Method
cpg	728.17	J/molxK	775.61	Joback Method
cpg	743.77	J/molxK	807.35	Joback Method
cpg	758.56	J/molxK	839.09	Joback Method
cpg	772.58	J/molxK	870.83	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=U299382&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299382&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</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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