

# Carbonic acid, but-2-yn-1-yl dodecyl ester

**Inchi:** InChI=1S/C17H30O3/c1-3-5-7-8-9-10-11-12-13-14-16-20-17(18)19-15-6-4-2/h3,5,7-16H2  
**InchiKey:** QPKGOSCWTKETIL-UHFFFAOYSA-N  
**Formula:** C17H30O3  
**SMILES:** CC#CCOC(=O)OCCCCCCCCCCCCC  
**Mol. weight [g/mol]:** 282.42

## Physical Properties

Property code	Value	Unit	Source
gf	-43.86	kJ/mol	Joback Method
hf	-498.93	kJ/mol	Joback Method
hfus	46.88	kJ/mol	Joback Method
hvap	67.15	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.084		Crippen Method
mvol	255.100	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	696.07	K	Joback Method
tc	876.96	K	Joback Method
tf	481.84	K	Joback Method
vc	0.992	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.50	J/mol×K	696.07	Joback Method
cpg	738.13	J/mol×K	726.22	Joback Method
cpg	754.92	J/mol×K	756.37	Joback Method
cpg	770.90	J/mol×K	786.51	Joback Method
cpg	786.06	J/mol×K	816.66	Joback Method
cpg	800.42	J/mol×K	846.81	Joback Method
cpg	813.98	J/mol×K	876.96	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=U383207&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383207&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>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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