

# Carbonic acid, but-3-en-1-yl dodecyl ester

**Inchi:** InChI=1S/C17H32O3/c1-3-5-7-8-9-10-11-12-13-14-16-20-17(18)19-15-6-4-2/h4H,2-3,5-1  
**InchiKey:** XMSNLFYAVWNTDG-UHFFFAOYSA-N  
**Formula:** C17H32O3  
**SMILES:** C=CCCOC(=O)OCCCCCCCCCCCCC  
**Mol. weight [g/mol]:** 284.43

## Physical Properties

Property code	Value	Unit	Source
gf	-158.82	kJ/mol	Joback Method
hf	-645.80	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	64.33	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.637		Crippen Method
mvol	259.400	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpol	1919.00		NIST Webbook
rinpol	1919.00		NIST Webbook
tb	683.75	K	Joback Method
tc	853.94	K	Joback Method
tf	373.98	K	Joback Method
vc	1.010	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.74	J/molxK	683.75	Joback Method
cpg	820.19	J/molxK	825.57	Joback Method
cpg	805.63	J/molxK	797.21	Joback Method
cpg	790.32	J/molxK	768.84	Joback Method
cpg	774.25	J/molxK	740.48	Joback Method
cpg	757.39	J/molxK	712.11	Joback Method
cpg	834.01	J/molxK	853.94	Joback Method
dvisc	0.0000875	Paxs	683.75	Joback Method

dvisc	0.0001157	Paxs	632.12	Joback Method
dvisc	0.0001607	Paxs	580.49	Joback Method
dvisc	0.0002381	Paxs	528.87	Joback Method
dvisc	0.0003840	Paxs	477.24	Joback Method
dvisc	0.0006954	Paxs	425.61	Joback Method
dvisc	0.0014838	Paxs	373.98	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=U383233&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383233&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>
<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>dvisc:</b>	Dynamic viscosity
<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>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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