

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

**Inchi:** InChI=1S/C16H30O3/c1-3-5-7-8-9-10-11-12-13-15-19-16(17)18-14-6-4-2/h4H,2-3,5-15H  
**InchiKey:** NICBOLAIDRXZLQ-UHFFFAOYSA-N  
**Formula:** C16H30O3  
**SMILES:** C=CCCOC(=O)OCCCCCCCCCCC  
**Mol. weight [g/mol]:** 270.41

## Physical Properties

Property code	Value	Unit	Source
gf	-167.24	kJ/mol	Joback Method
hf	-625.16	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	62.11	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	5.247		Crippen Method
mvol	245.310	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
tb	660.87	K	Joback Method
tc	830.71	K	Joback Method
tf	362.71	K	Joback Method
vc	0.955	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.38	J/molxK	660.87	Joback Method
cpg	700.56	J/molxK	689.18	Joback Method
cpg	717.00	J/molxK	717.48	Joback Method
cpg	732.69	J/molxK	745.79	Joback Method
cpg	747.66	J/molxK	774.10	Joback Method
cpg	761.91	J/molxK	802.40	Joback Method
cpg	775.46	J/molxK	830.71	Joback Method
dvisc	0.0016121	Paxs	362.71	Joback Method

dvisc	0.0007654	Paxs	412.40	Joback Method
dvisc	0.0004265	Paxs	462.10	Joback Method
dvisc	0.0002663	Paxs	511.79	Joback Method
dvisc	0.0001807	Paxs	561.48	Joback Method
dvisc	0.0001306	Paxs	611.18	Joback Method
dvisc	0.0000991	Paxs	660.87	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=U383232&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383232&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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