

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

Inchi:	InChI=1S/C21H40O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-20-24-21(22)23-19-6-4-2
InchiKey:	OTRORGODLHWRCU-UHFFFAOYSA-N
Formula:	C21H40O3
SMILES:	C=CCCOC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	340.54

## Physical Properties

Property code	Value	Unit	Source
gf	-125.14	kJ/mol	Joback Method
hf	-728.36	kJ/mol	Joback Method
hfus	52.84	kJ/mol	Joback Method
hvap	73.24	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	7.197		Crippen Method
mvol	315.760	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
rinpol	2317.00		NIST Webbook
rinpol	2317.00		NIST Webbook
tb	775.27	K	Joback Method
tc	952.22	K	Joback Method
tf	419.06	K	Joback Method
vc	1.234	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.22	J/molxK	775.27	Joback Method
cpg	995.64	J/molxK	804.76	Joback Method
cpg	1014.07	J/molxK	834.25	Joback Method
cpg	1031.53	J/molxK	863.74	Joback Method
cpg	1048.05	J/molxK	893.23	Joback Method
cpg	1063.64	J/molxK	922.72	Joback Method
cpg	1078.32	J/molxK	952.22	Joback Method
dvisc	0.0010054	Paxs	419.06	Joback Method

dvisc	0.0004502	Paxs	478.43	Joback Method
dvisc	0.0002407	Paxs	537.80	Joback Method
dvisc	0.0001458	Paxs	597.16	Joback Method
dvisc	0.0000967	Paxs	656.53	Joback Method
dvisc	0.0000686	Paxs	715.90	Joback Method
dvisc	0.0000513	Paxs	775.27	Joback Method

## Sources

<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>
<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=U383237&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383237&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>

## Legend

<b>cp<sub>g</sub>:</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>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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