

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

<b>Inchi:</b>	InChI=1S/C11H20O3/c1-3-5-7-8-10-14-11(12)13-9-6-4-2/h4H,2-3,5-10H2,1H3
<b>InchiKey:</b>	DEHFDEBDQQOIHU-UHFFFAOYSA-N
<b>Formula:</b>	C11H20O3
<b>SMILES:</b>	C=CCCOC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	200.27

## Physical Properties

Property code	Value	Unit	Source
gf	-209.34	kJ/mol	Joback Method
hf	-521.96	kJ/mol	Joback Method
hfus	26.94	kJ/mol	Joback Method
hvap	50.98	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.296		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1338.00		NIST Webbook
rinpol	1338.00		NIST Webbook
tb	546.47	K	Joback Method
tc	719.93	K	Joback Method
tf	306.36	K	Joback Method
vc	0.674	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.56	J/molxK	546.47	Joback Method
cpg	488.21	J/molxK	691.02	Joback Method
cpg	476.16	J/molxK	662.11	Joback Method
cpg	463.57	J/molxK	633.20	Joback Method
cpg	450.44	J/molxK	604.29	Joback Method
cpg	436.77	J/molxK	575.38	Joback Method
cpg	499.74	J/molxK	719.93	Joback Method
dvisc	0.0001707	Paxs	546.47	Joback Method

dvisc	0.0002205	Paxs	506.45	Joback Method
dvisc	0.0002977	Paxs	466.43	Joback Method
dvisc	0.0004251	Paxs	426.42	Joback Method
dvisc	0.0006537	Paxs	386.40	Joback Method
dvisc	0.0011102	Paxs	346.38	Joback Method
dvisc	0.0021653	Paxs	306.36	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=U383227&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383227&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.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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