

# Carbonic acid, hexadecyl prop-1-en-2-yl ester

**Inchi:** InChI=1S/C20H38O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-20(21)23-19(2)3/h2  
**InchiKey:** NPIONMYPQNAYPB-UHFFFAOYSA-N  
**Formula:** C20H38O3  
**SMILES:** C=C(C)OC(=O)OCCCCCCCCCCCCCCCCC  
**Mol. weight [g/mol]:** 326.51

## Physical Properties

Property code	Value	Unit	Source
gf	-142.11	kJ/mol	Joback Method
hf	-717.51	kJ/mol	Joback Method
hfus	48.94	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	7.154		Crippen Method
mvol	301.670	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	752.27	K	Joback Method
tc	927.58	K	Joback Method
tf	393.83	K	Joback Method
vc	1.179	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.25	J/mol×K	752.27	Joback Method
cpg	934.31	J/mol×K	781.49	Joback Method
cpg	952.43	J/mol×K	810.71	Joback Method
cpg	969.63	J/mol×K	839.93	Joback Method
cpg	985.93	J/mol×K	869.15	Joback Method
cpg	1001.35	J/mol×K	898.36	Joback Method
cpg	1015.91	J/mol×K	927.58	Joback Method

# Sources

<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>
<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=U382903&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382903&amp;Units=SI</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>hvp:</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>rinp:</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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