

# Carbonic acid, 2-ethylhexyl hexadecyl ester

**Inchi:** InChI=1S/C25H50O3/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-22-27-25(26)28-23-24  
**InchiKey:** KAPWKWLEYXPMTF-UHFFFAOYSA-N  
**Formula:** C25H50O3  
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)OCC(CC)CCCC  
**Mol. weight [g/mol]:** 398.66

## Physical Properties

Property code	Value	Unit	Source
gf	-181.74	kJ/mol	Joback Method
hf	-941.63	kJ/mol	Joback Method
hfus	60.96	kJ/mol	Joback Method
hvap	82.42	kJ/mol	Joback Method
log10ws	-8.97		Crippen Method
logp	8.837		Crippen Method
mvol	376.420	ml/mol	McGowan Method
pc	779.81	kPa	Joback Method
rinpol	2638.00		NIST Webbook
rinpol	2638.00		NIST Webbook
tb	869.67	K	Joback Method
tc	1065.59	K	Joback Method
tf	450.90	K	Joback Method
vc	1.472	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1255.49	J/molxK	869.67	Joback Method
cpg	1277.60	J/molxK	902.32	Joback Method
cpg	1298.34	J/molxK	934.98	Joback Method
cpg	1317.73	J/molxK	967.63	Joback Method
cpg	1335.81	J/molxK	1000.28	Joback Method
cpg	1352.62	J/molxK	1032.94	Joback Method
cpg	1368.19	J/molxK	1065.59	Joback Method
dvisc	0.0007426	Paxs	450.90	Joback Method

dvisc	0.0002875	Paxs	520.69	Joback Method
dvisc	0.0001393	Paxs	590.49	Joback Method
dvisc	0.0000786	Paxs	660.28	Joback Method
dvisc	0.0000495	Paxs	730.08	Joback Method
dvisc	0.0000338	Paxs	799.88	Joback Method
dvisc	0.0000246	Paxs	869.67	Joback Method

## Sources

<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>
<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=U383143&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383143&amp;Units=SI</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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