

# cis-Cyclohex-4-en-1,2-dicarboxylic acid, hexyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C27H48O4/c1-3-5-7-9-10-11-12-13-14-15-19-23-31-27(29)25-21-17-16-20-24(
<b>InchiKey:</b>	NRTJYIGJSBPBKL-UHFFFAOYSA-N
<b>Formula:</b>	C27H48O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	436.67

## Physical Properties

Property code	Value	Unit	Source
gf	-244.68	kJ/mol	Joback Method
hf	-998.45	kJ/mol	Joback Method
hfus	65.39	kJ/mol	Joback Method
hvap	94.42	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.546		Crippen Method
mvol	391.010	ml/mol	McGowan Method
pc	811.68	kPa	Joback Method
rinpol	2982.00		NIST Webbook
rinpol	2982.00		NIST Webbook
tb	983.78	K	Joback Method
tc	1206.49	K	Joback Method
tf	542.27	K	Joback Method
vc	1.514	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1378.93	J/molxK	983.78	Joback Method
cpg	1458.95	J/molxK	1169.37	Joback Method
cpg	1446.51	J/molxK	1132.25	Joback Method
cpg	1432.34	J/molxK	1095.13	Joback Method
cpg	1416.38	J/molxK	1058.02	Joback Method
cpg	1398.60	J/molxK	1020.90	Joback Method
cpg	1469.72	J/molxK	1206.49	Joback Method
dvisc	0.0000279	Paxs	983.78	Joback Method

dvisc	0.0000368	Paxs	910.20	Joback Method
dvisc	0.0000509	Paxs	836.61	Joback Method
dvisc	0.0000751	Paxs	763.03	Joback Method
dvisc	0.0001203	Paxs	689.44	Joback Method
dvisc	0.0002157	Paxs	615.86	Joback Method
dvisc	0.0004533	Paxs	542.27	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=U382688&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382688&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</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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