

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

<b>Inchi:</b>	InChI=1S/C29H52O4/c1-4-7-9-10-11-12-13-14-15-16-19-23-32-28(30)26-21-17-18-22-27
<b>InchiKey:</b>	JSKYHKQIDMKTLN-UHFFFAOYSA-N
<b>Formula:</b>	C29H52O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CCCC
<b>Mol. weight [g/mol]:</b>	464.72

## Physical Properties

Property code	Value	Unit	Source
gf	-230.28	kJ/mol	Joback Method
hf	-1045.01	kJ/mol	Joback Method
hfus	67.05	kJ/mol	Joback Method
hvap	98.48	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.183		Crippen Method
mvol	419.190	ml/mol	McGowan Method
pc	732.84	kPa	Joback Method
rinpol	3092.00		NIST Webbook
rinpol	3092.00		NIST Webbook
tb	1029.10	K	Joback Method
tc	1267.06	K	Joback Method
tf	549.81	K	Joback Method
vc	1.619	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1507.59	J/molxK	1029.10	Joback Method
cpg	1527.59	J/molxK	1068.76	Joback Method
cpg	1545.40	J/molxK	1108.42	Joback Method
cpg	1561.09	J/molxK	1148.08	Joback Method
cpg	1574.73	J/molxK	1187.74	Joback Method
cpg	1586.39	J/molxK	1227.40	Joback Method
cpg	1596.14	J/molxK	1267.06	Joback Method
dvisc	0.0003927	Paxs	549.81	Joback Method

dvisc	0.0001713	Paxs	629.69	Joback Method
dvisc	0.0000900	Paxs	709.57	Joback Method
dvisc	0.0000539	Paxs	789.45	Joback Method
dvisc	0.0000355	Paxs	869.34	Joback Method
dvisc	0.0000250	Paxs	949.22	Joback Method
dvisc	0.0000187	Paxs	1029.10	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=U382640&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382640&amp;Units=SI</a>
<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.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>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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