

# cis-Cyclohex-4-en-1,2-dicarboxylic acid, dodecyl 2-ethylbutyl ester

Inchi:	InChI=1S/C26H46O4/c1-4-7-8-9-10-11-12-13-14-17-20-29-25(27)23-18-15-16-19-24(23)
InchiKey:	DSRYLCDPJCQCGM-UHFFFAOYSA-N
Formula:	C26H46O4
SMILES:	CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CC
Mol. weight [g/mol]:	422.64

## Physical Properties

Property code	Value	Unit	Source
gf	-255.54	kJ/mol	Joback Method
hf	-983.09	kJ/mol	Joback Method
hfus	59.27	kJ/mol	Joback Method
hvap	91.81	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	7.012		Crippen Method
mvol	376.920	ml/mol	McGowan Method
pc	862.01	kPa	Joback Method
rinpol	2834.00		NIST Webbook
rinpol	2834.00		NIST Webbook
tb	960.46	K	Joback Method
tc	1176.05	K	Joback Method
tf	516.00	K	Joback Method
vc	1.452	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.49	J/molxK	960.46	Joback Method
cpg	1334.86	J/molxK	996.39	Joback Method
cpg	1352.46	J/molxK	1032.32	Joback Method
cpg	1368.34	J/molxK	1068.26	Joback Method
cpg	1382.55	J/molxK	1104.19	Joback Method
cpg	1395.13	J/molxK	1140.12	Joback Method
cpg	1406.12	J/molxK	1176.05	Joback Method
dvisc	0.0005760	Paxs	516.00	Joback Method

dvisc	0.0002572	Paxs	590.08	Joback Method
dvisc	0.0001375	Paxs	664.15	Joback Method
dvisc	0.0000833	Paxs	738.23	Joback Method
dvisc	0.0000553	Paxs	812.31	Joback Method
dvisc	0.0000394	Paxs	886.38	Joback Method
dvisc	0.0000295	Paxs	960.46	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=U382814&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382814&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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