

# cis-Cyclohex-4-en-1,2-dicarboxylic acid, isoheptyl undecyl ester

<b>Inchi:</b>	InChI=1S/C25H44O4/c1-4-5-6-7-8-9-10-11-14-19-28-24(26)22-17-12-13-18-23(22)25(27)
<b>InchiKey:</b>	AZVHMHPLYOFQDE-UHFFFAOYSA-N
<b>Formula:</b>	C25H44O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCC(C)C
<b>Mol. weight [g/mol]:</b>	408.61

## Physical Properties

Property code	Value	Unit	Source
gf	-263.96	kJ/mol	Joback Method
hf	-962.45	kJ/mol	Joback Method
hfus	56.68	kJ/mol	Joback Method
hvap	89.58	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.622		Crippen Method
mvol	362.830	ml/mol	McGowan Method
pc	912.73	kPa	Joback Method
rinpol	2740.00		NIST Webbook
rinpol	2740.00		NIST Webbook
tb	937.58	K	Joback Method
tc	1147.94	K	Joback Method
tf	504.73	K	Joback Method
vc	1.395	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.08	J/molxK	937.58	Joback Method
cpg	1331.90	J/molxK	1112.88	Joback Method
cpg	1319.10	J/molxK	1077.82	Joback Method
cpg	1304.75	J/molxK	1042.76	Joback Method
cpg	1288.83	J/molxK	1007.70	Joback Method
cpg	1271.28	J/molxK	972.64	Joback Method
cpg	1343.20	J/molxK	1147.94	Joback Method
dvisc	0.0000342	Paxs	937.58	Joback Method

dvisc	0.0000456	Paxs	865.44	Joback Method
dvisc	0.0000639	Paxs	793.30	Joback Method
dvisc	0.0000960	Paxs	721.15	Joback Method
dvisc	0.0001576	Paxs	649.01	Joback Method
dvisc	0.0002931	Paxs	576.87	Joback Method
dvisc	0.0006508	Paxs	504.73	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U382686&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382686&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.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>

## 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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