

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

Inchi:	InChI=1S/C22H38O4/c1-4-5-6-7-8-11-16-25-21(23)19-14-9-10-15-20(19)22(24)26-17-12
InchiKey:	LGUUOHIIIBBPLKC-UHFFFAOYSA-N
Formula:	C22H38O4
SMILES:	CCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]:	366.53

## Physical Properties

Property code	Value	Unit	Source
gf	-289.22	kJ/mol	Joback Method
hf	-900.53	kJ/mol	Joback Method
hfus	48.91	kJ/mol	Joback Method
hvap	82.90	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.452		Crippen Method
mvol	320.560	ml/mol	McGowan Method
pc	1094.99	kPa	Joback Method
rinpol	2440.00		NIST Webbook
rinpol	2440.00		NIST Webbook
tb	868.94	K	Joback Method
tc	1069.26	K	Joback Method
tf	470.92	K	Joback Method
vc	1.228	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.43	J/molxK	868.94	Joback Method
cpg	1083.28	J/molxK	902.33	Joback Method
cpg	1100.70	J/molxK	935.71	Joback Method
cpg	1116.73	J/molxK	969.10	Joback Method
cpg	1131.38	J/molxK	1002.48	Joback Method
cpg	1144.69	J/molxK	1035.87	Joback Method
cpg	1156.67	J/molxK	1069.26	Joback Method
dvisc	0.0009203	Paxs	470.92	Joback Method

dvisc	0.0004261	Paxs	537.26	Joback Method
dvisc	0.0002336	Paxs	603.59	Joback Method
dvisc	0.0001443	Paxs	669.93	Joback Method
dvisc	0.0000972	Paxs	736.27	Joback Method
dvisc	0.0000699	Paxs	802.60	Joback Method
dvisc	0.0000529	Paxs	868.94	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=U382684&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382684&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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