

# cis-Cyclohex-4-en-1,2-dicarboxylic acid, 2-methylbutyl pentyl ester

<b>Inchi:</b>	InChI=1S/C18H30O4/c1-4-6-9-12-21-17(19)15-10-7-8-11-16(15)18(20)22-13-14(3)5-2/h
<b>InchiKey:</b>	WAYRRKZSEKLNQA-UHFFFAOYSA-N
<b>Formula:</b>	C18H30O4
<b>SMILES:</b>	CCCCCOC(=O)C1CC=CCC1C(=O)OCC(C)CC
<b>Mol. weight [g/mol]:</b>	310.43

## Physical Properties

Property code	Value	Unit	Source
gf	-322.90	kJ/mol	Joback Method
hf	-817.97	kJ/mol	Joback Method
hfus	38.55	kJ/mol	Joback Method
hvap	74.00	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.891		Crippen Method
mvol	264.200	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook
tb	777.42	K	Joback Method
tc	975.18	K	Joback Method
tf	425.84	K	Joback Method
vc	1.004	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.66	J/molxK	777.42	Joback Method
cpg	841.13	J/molxK	810.38	Joback Method
cpg	858.38	J/molxK	843.34	Joback Method
cpg	874.42	J/molxK	876.30	Joback Method
cpg	889.25	J/molxK	909.26	Joback Method
cpg	902.89	J/molxK	942.22	Joback Method
cpg	915.36	J/molxK	975.18	Joback Method
dvisc	0.0013807	Paxs	425.84	Joback Method

dvisc	0.0006672	Paxs	484.44	Joback Method
dvisc	0.0003772	Paxs	543.03	Joback Method
dvisc	0.0002383	Paxs	601.63	Joback Method
dvisc	0.0001633	Paxs	660.23	Joback Method
dvisc	0.0001191	Paxs	718.82	Joback Method
dvisc	0.0000910	Paxs	777.42	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=U382694&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382694&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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