

# 1,2-Cyclohexanedicarboxylic acid, isobutyl tetradecyl ester

Inchi:	InChI=1S/C26H48O4/c1-4-5-6-7-8-9-10-11-12-13-14-17-20-29-25(27)23-18-15-16-19-24
InchiKey:	HNIYTQZUWSFMTE-UHFFFAOYSA-N
Formula:	C26H48O4
SMILES:	CCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]:	424.66

## Physical Properties

Property code	Value	Unit	Source
gf	-285.50	kJ/mol	Joback Method
hf	-1040.87	kJ/mol	Joback Method
hfus	58.05	kJ/mol	Joback Method
hvap	91.51	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	7.236		Crippen Method
mvol	381.220	ml/mol	McGowan Method
pc	844.07	kPa	Joback Method
rinpol	2902.00		NIST Webbook
rinpol	2902.00		NIST Webbook
tb	961.30	K	Joback Method
tc	1177.22	K	Joback Method
tf	515.24	K	Joback Method
vc	1.466	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.53	J/molxK	961.30	Joback Method
cpg	1366.57	J/molxK	997.29	Joback Method
cpg	1384.77	J/molxK	1033.27	Joback Method
cpg	1401.18	J/molxK	1069.26	Joback Method
cpg	1415.85	J/molxK	1105.24	Joback Method
cpg	1428.81	J/molxK	1141.23	Joback Method
cpg	1440.11	J/molxK	1177.22	Joback Method
dvisc	0.0005807	Paxs	515.24	Joback Method

dvisc	0.0002521	Paxs	589.58	Joback Method
dvisc	0.0001319	Paxs	663.93	Joback Method
dvisc	0.0000787	Paxs	738.27	Joback Method
dvisc	0.0000516	Paxs	812.61	Joback Method
dvisc	0.0000363	Paxs	886.96	Joback Method
dvisc	0.0000269	Paxs	961.30	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=U339434&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339434&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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