

# 1,2-Cyclohexanedicarboxylic acid, 2-biphenyl isohexyl ester

Inchi:	InChI=1S/C26H32O4/c1-19(2)11-10-18-29-25(27)22-15-6-7-16-23(22)26(28)30-24-17-9-
InchiKey:	AANLGCSUWATOMO-UHFFFAOYSA-N
Formula:	C26H32O4
SMILES:	CC(C)CCCOC(=O)C1CCCCC1C(=O)Oc1cccc1-c1cccc1
Mol. weight [g/mol]:	408.53

## Physical Properties

Property code	Value	Unit	Source
gf	-70.31	kJ/mol	Joback Method
hf	-579.28	kJ/mol	Joback Method
hfus	45.75	kJ/mol	Joback Method
hvap	96.73	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	6.045		Crippen Method
mcvol	333.700	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2922.00		NIST Webbook
rinpol	2922.00		NIST Webbook
tb	1019.64	K	Joback Method
tc	1260.97	K	Joback Method
tf	580.60	K	Joback Method
vc	1.250	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1135.48	J/molxK	1019.64	Joback Method
cpg	1187.22	J/molxK	1220.75	Joback Method
cpg	1180.42	J/molxK	1180.53	Joback Method
cpg	1171.91	J/molxK	1140.30	Joback Method
cpg	1161.63	J/molxK	1100.08	Joback Method
cpg	1149.51	J/molxK	1059.86	Joback Method
cpg	1192.38	J/molxK	1260.97	Joback Method
dvisc	0.0000298	Paxs	1019.64	Joback Method

dvisc	0.0000386	Paxs	946.47	Joback Method
dvisc	0.0000523	Paxs	873.29	Joback Method
dvisc	0.0000748	Paxs	800.12	Joback Method
dvisc	0.0001151	Paxs	726.95	Joback Method
dvisc	0.0001950	Paxs	653.77	Joback Method
dvisc	0.0003774	Paxs	580.60	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=U339596&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339596&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>

## 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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