

# 1,2-Cyclohexanedicarboxylic acid, dicyclohexyl ester

**Inchi:** InChI=1S/C20H32O4/c21-19(23-15-9-3-1-4-10-15)17-13-7-8-14-18(17)20(22)24-16-11-5  
**InchiKey:** VKPGBQAXQBOSCY-UHFFFAOYSA-N  
**Formula:** C20H32O4  
**SMILES:** O=C(OC1CCCCC1)C1CCCCC1C(=O)OC1CCCCC1  
**Mol. weight [g/mol]:** 336.47

## Physical Properties

Property code	Value	Unit	Source
gf	-284.68	kJ/mol	Joback Method
hf	-803.11	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	79.40	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.545		Crippen Method
mvol	274.960	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	2480.00		NIST Webbook
rinpol	2480.00		NIST Webbook
tb	863.56	K	Joback Method
tc	1103.01	K	Joback Method
tf	477.38	K	Joback Method
vc	1.002	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.67	J/molxK	863.56	Joback Method
cpg	985.27	J/molxK	903.47	Joback Method
cpg	1004.56	J/molxK	943.38	Joback Method
cpg	1021.60	J/molxK	983.28	Joback Method
cpg	1036.41	J/molxK	1023.19	Joback Method
cpg	1049.03	J/molxK	1063.10	Joback Method
cpg	1059.51	J/molxK	1103.01	Joback Method
dvisc	0.0013290	Paxs	477.38	Joback Method

dvisc	0.0006213	Paxs	541.74	Joback Method
dvisc	0.0003414	Paxs	606.11	Joback Method
dvisc	0.0002104	Paxs	670.47	Joback Method
dvisc	0.0001412	Paxs	734.83	Joback Method
dvisc	0.0001010	Paxs	799.20	Joback Method
dvisc	0.0000760	Paxs	863.56	Joback Method

## Sources

<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=U339766&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339766&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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