

# 1,2-Cyclohexanedicarboxylic acid, dicyclohexylmethyl ester

Inchi:	InChI=1S/C22H36O4/c23-21(25-15-17-9-3-1-4-10-17)19-13-7-8-14-20(19)22(24)26-16-1
InchiKey:	ITEOMAHCDRDDLQ-UHFFFAOYSA-N
Formula:	C22H36O4
SMILES:	O=C(OCC1CCCCC1)C1CCCCC1C(=O)OCC1CCCCC1
Mol. weight [g/mol]:	364.52

## Physical Properties

Property code	Value	Unit	Source
gf	-267.84	kJ/mol	Joback Method
hf	-844.39	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	83.86	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	5.040		Crippen Method
mvol	303.140	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	2713.00		NIST Webbook
rinpol	2713.00		NIST Webbook
tb	909.32	K	Joback Method
tc	1143.22	K	Joback Method
tf	499.92	K	Joback Method
vc	1.113	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.12	J/molxK	909.32	Joback Method
cpg	1107.60	J/molxK	948.30	Joback Method
cpg	1125.80	J/molxK	987.29	Joback Method
cpg	1141.77	J/molxK	1026.27	Joback Method
cpg	1155.54	J/molxK	1065.25	Joback Method
cpg	1167.17	J/molxK	1104.24	Joback Method
cpg	1176.69	J/molxK	1143.22	Joback Method
dvisc	0.0010562	Paxs	499.92	Joback Method

dvisc	0.0004845	Paxs	568.15	Joback Method
dvisc	0.0002627	Paxs	636.39	Joback Method
dvisc	0.0001604	Paxs	704.62	Joback Method
dvisc	0.0001068	Paxs	772.85	Joback Method
dvisc	0.0000760	Paxs	841.09	Joback Method
dvisc	0.0000569	Paxs	909.32	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=U339749&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339749&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>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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