

# 1,2-Cyclohexanedicarboxylic acid, cyclohexylmethyl nonyl ester

**Inchi:** InChI=1S/C24H42O4/c1-2-3-4-5-6-7-13-18-27-23(25)21-16-11-12-17-22(21)24(26)28-19  
**InchiKey:** UXPSBBXEVRMWFU-UHFFFAOYSA-N  
**Formula:** C24H42O4  
**SMILES:** CCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC1CCCCC1  
**Mol. weight [g/mol]:** 394.59

## Physical Properties

Property code	Value	Unit	Source
gf	-275.45	kJ/mol	Joback Method
hf	-939.99	kJ/mol	Joback Method
hfus	48.23	kJ/mol	Joback Method
hvap	87.88	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	6.210		Crippen Method
mvol	342.180	ml/mol	McGowan Method
pc	1072.87	kPa	Joback Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook
tb	935.53	K	Joback Method
tc	1150.78	K	Joback Method
tf	515.08	K	Joback Method
vc	1.292	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.77	J/molxK	935.53	Joback Method
cpg	1294.61	J/molxK	1114.91	Joback Method
cpg	1282.44	J/molxK	1079.03	Joback Method
cpg	1268.51	J/molxK	1043.16	Joback Method
cpg	1252.77	J/molxK	1007.28	Joback Method
cpg	1235.21	J/molxK	971.41	Joback Method
cpg	1305.07	J/molxK	1150.78	Joback Method
dvisc	0.0000411	Paxs	935.53	Joback Method

dvisc	0.0000547	Paxs	865.45	Joback Method
dvisc	0.0000766	Paxs	795.38	Joback Method
dvisc	0.0001145	Paxs	725.30	Joback Method
dvisc	0.0001865	Paxs	655.23	Joback Method
dvisc	0.0003414	Paxs	585.15	Joback Method
dvisc	0.0007366	Paxs	515.08	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=U339743&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339743&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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