

# 1,2-Cyclohexanedicarboxylic acid, pentyl 3-phenylpropyl ester

Inchi:	InChI=1S/C22H32O4/c1-2-3-9-16-25-21(23)19-14-7-8-15-20(19)22(24)26-17-10-13-18-1
InchiKey:	XNGQHDLQLBWWOB-UHFFFAOYSA-N
Formula:	C22H32O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	360.49

## Physical Properties

Property code	Value	Unit	Source
gf	-204.33	kJ/mol	Joback Method
hf	-716.50	kJ/mol	Joback Method
hfus	45.26	kJ/mol	Joback Method
hvap	85.27	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.702		Crippen Method
mvol	301.100	ml/mol	McGowan Method
pc	1336.86	kPa	Joback Method
rinpol	2648.00		NIST Webbook
rinpol	2648.00		NIST Webbook
tb	896.90	K	Joback Method
tc	1113.61	K	Joback Method
tf	511.58	K	Joback Method
vc	1.139	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.41	J/molxK	896.90	Joback Method
cpg	1014.69	J/molxK	933.02	Joback Method
cpg	1030.39	J/molxK	969.14	Joback Method
cpg	1044.54	J/molxK	1005.25	Joback Method
cpg	1057.18	J/molxK	1041.37	Joback Method
cpg	1068.35	J/molxK	1077.49	Joback Method
cpg	1078.07	J/molxK	1113.61	Joback Method
dvisc	0.0006985	Paxs	511.58	Joback Method

dvisc	0.0003609	Paxs	575.80	Joback Method
dvisc	0.0002129	Paxs	640.02	Joback Method
dvisc	0.0001383	Paxs	704.24	Joback Method
dvisc	0.0000965	Paxs	768.46	Joback Method
dvisc	0.0000712	Paxs	832.68	Joback Method
dvisc	0.0000549	Paxs	896.90	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=U339496&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339496&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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