

# 1,2-Cyclohexanedicarboxylic acid, dodecyl 3-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C27H42O4/c1-3-4-5-6-7-8-9-10-11-14-20-30-26(28)24-18-12-13-19-25(24)27(2)
<b>InchiKey:</b>	PTDNNQMIUOANCB-UHFFFAOYSA-N
<b>Formula:</b>	C27H42O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	430.62

## Physical Properties

Property code	Value	Unit	Source
gf	-171.86	kJ/mol	Joback Method
hf	-831.17	kJ/mol	Joback Method
hfus	57.82	kJ/mol	Joback Method
hvap	97.07	kJ/mol	Joback Method
log10ws	-8.07		Crippen Method
logp	7.171		Crippen Method
mcvol	371.550	ml/mol	McGowan Method
pc	958.51	kPa	Joback Method
rinpol	3147.00		NIST Webbook
tb	1016.28	K	Joback Method
tc	1244.40	K	Joback Method
tf	580.45	K	Joback Method
vc	1.419	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1305.23	J/molxK	1016.28	Joback Method
cpg	1370.22	J/molxK	1206.38	Joback Method
cpg	1360.79	J/molxK	1168.36	Joback Method
cpg	1349.64	J/molxK	1130.34	Joback Method
cpg	1336.69	J/molxK	1092.32	Joback Method
cpg	1321.91	J/molxK	1054.30	Joback Method
cpg	1377.97	J/molxK	1244.40	Joback Method
dvisc	0.0000271	Paxs	1016.28	Joback Method
dvisc	0.0000352	Paxs	943.64	Joback Method

dvisc	0.0000477	Paxs	871.00	Joback Method
dvisc	0.0000684	Paxs	798.37	Joback Method
dvisc	0.0001053	Paxs	725.73	Joback Method
dvisc	0.0001786	Paxs	653.09	Joback Method
dvisc	0.0003459	Paxs	580.45	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=U339839&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339839&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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