

# 1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylphenyl dodecyl ester

**Inchi:** InChI=1S/C28H44O4/c1-4-5-6-7-8-9-10-11-12-15-18-31-27(29)25-16-13-14-17-26(25)28  
**InchiKey:** GNNGLPSVEPCRRX-UHFFFAOYSA-N  
**Formula:** C28H44O4  
**SMILES:** CCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(C)cc(C)c1  
**Mol. weight [g/mol]:** 444.65

## Physical Properties

Property code	Value	Unit	Source
gf	-173.07	kJ/mol	Joback Method
hf	-863.28	kJ/mol	Joback Method
hfus	60.02	kJ/mol	Joback Method
hvap	99.95	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	7.479		Crippen Method
mcvol	385.640	ml/mol	McGowan Method
pc	895.87	kPa	Joback Method
rinpol	3223.00		NIST Webbook
tb	1044.14	K	Joback Method
tc	1278.45	K	Joback Method
tf	604.24	K	Joback Method
vc	1.476	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1367.10	J/molxK	1044.14	Joback Method
cpg	1429.13	J/molxK	1239.40	Joback Method
cpg	1420.59	J/molxK	1200.35	Joback Method
cpg	1410.18	J/molxK	1161.30	Joback Method
cpg	1397.83	J/molxK	1122.24	Joback Method
cpg	1383.48	J/molxK	1083.19	Joback Method
cpg	1435.83	J/molxK	1278.45	Joback Method
dvisc	0.0000240	Paxs	1044.14	Joback Method
dvisc	0.0000308	Paxs	970.82	Joback Method

dvisc	0.0000414	Paxs	897.51	Joback Method
dvisc	0.0000585	Paxs	824.19	Joback Method
dvisc	0.0000884	Paxs	750.87	Joback Method
dvisc	0.0001462	Paxs	677.56	Joback Method
dvisc	0.0002732	Paxs	604.24	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U339621&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339621&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mccvol:</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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