

# 1,2-Cyclohexanedicarboxylic acid, cyclohex-3-enylmethyl dodecyl ester

Inchi:	InChI=1S/C27H46O4/c1-2-3-4-5-6-7-8-9-10-16-21-30-26(28)24-19-14-15-20-25(24)27(29)
InchiKey:	SWISUTBBSSMGTL-UHFFFAOYSA-N
Formula:	C27H46O4
SMILES:	CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC1CC=CCC1
Mol. weight [g/mol]:	434.65

## Physical Properties

Property code	Value	Unit	Source
gf	-220.23	kJ/mol	Joback Method
hf	-944.13	kJ/mol	Joback Method
hfus	57.22	kJ/mol	Joback Method
hvap	94.85	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	7.156		Crippen Method
mvol	380.150	ml/mol	McGowan Method
pc	915.50	kPa	Joback Method
rinpol	3144.00		NIST Webbook
rinpol	3144.00		NIST Webbook
tb	1003.33	K	Joback Method
tc	1228.48	K	Joback Method
tf	549.65	K	Joback Method
vc	1.446	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1374.56	J/molxK	1003.33	Joback Method
cpg	1392.92	J/molxK	1040.85	Joback Method
cpg	1409.25	J/molxK	1078.38	Joback Method
cpg	1423.58	J/molxK	1115.90	Joback Method
cpg	1435.99	J/molxK	1153.43	Joback Method
cpg	1446.53	J/molxK	1190.95	Joback Method
cpg	1455.25	J/molxK	1228.48	Joback Method
dvisc	0.0005076	Paxs	549.65	Joback Method

dvisc	0.0002353	Paxs	625.26	Joback Method
dvisc	0.0001287	Paxs	700.88	Joback Method
dvisc	0.0000792	Paxs	776.49	Joback Method
dvisc	0.0000531	Paxs	852.10	Joback Method
dvisc	0.0000380	Paxs	927.72	Joback Method
dvisc	0.0000286	Paxs	1003.33	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=U339874&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339874&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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