

# 1,2-Cyclohexanedicarboxylic acid, 2-methylbutyl tetradecyl ester

Inchi:	InChI=1S/C27H50O4/c1-4-6-7-8-9-10-11-12-13-14-15-18-21-30-26(28)24-19-16-17-20-2
InchiKey:	MBDVIKUCQJDRHA-UHFFFAOYSA-N
Formula:	C27H50O4
SMILES:	CCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC(C)CC
Mol. weight [g/mol]:	438.68

## Physical Properties

Property code	Value	Unit	Source
gf	-277.08	kJ/mol	Joback Method
hf	-1061.51	kJ/mol	Joback Method
hfus	60.64	kJ/mol	Joback Method
hvap	93.74	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	7.626		Crippen Method
mcvol	395.310	ml/mol	McGowan Method
pc	798.89	kPa	Joback Method
rinpol	3003.00		NIST Webbook
rinpol	3003.00		NIST Webbook
tb	984.18	K	Joback Method
tc	1206.59	K	Joback Method
tf	526.51	K	Joback Method
vc	1.522	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.73	J/molxK	984.18	Joback Method
cpg	1430.94	J/molxK	1021.25	Joback Method
cpg	1449.19	J/molxK	1058.32	Joback Method
cpg	1465.52	J/molxK	1095.39	Joback Method
cpg	1480.00	J/molxK	1132.45	Joback Method
cpg	1492.66	J/molxK	1169.52	Joback Method
cpg	1503.56	J/molxK	1206.59	Joback Method
dvisc	0.0005103	Paxs	526.51	Joback Method

dvisc	0.0002198	Paxs	602.79	Joback Method
dvisc	0.0001144	Paxs	679.07	Joback Method
dvisc	0.0000680	Paxs	755.35	Joback Method
dvisc	0.0000444	Paxs	831.62	Joback Method
dvisc	0.0000312	Paxs	907.90	Joback Method
dvisc	0.0000231	Paxs	984.18	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=U339552&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339552&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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