

# 1,2-Cyclohexanedicarboxylic acid, decyl 2-methoxyethyl ester

Inchi:	InChI=1S/C21H38O5/c1-3-4-5-6-7-8-9-12-15-25-20(22)18-13-10-11-14-19(18)21(23)26-
InchiKey:	NLSNGRHQPLPLIL-UHFFFAOYSA-N
Formula:	C21H38O5
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOC
Mol. weight [g/mol]:	370.52

## Physical Properties

Property code	Value	Unit	Source
gf	-430.16	kJ/mol	Joback Method
hf	-1064.61	kJ/mol	Joback Method
hfus	49.81	kJ/mol	Joback Method
hvap	83.18	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.666		Crippen Method
mvol	316.640	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	2537.00		NIST Webbook
rinpol	2537.00		NIST Webbook
tb	869.76	K	Joback Method
tc	1068.88	K	Joback Method
tf	496.12	K	Joback Method
vc	1.210	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.78	J/molxK	869.76	Joback Method
cpg	1081.56	J/molxK	902.95	Joback Method
cpg	1098.86	J/molxK	936.13	Joback Method
cpg	1114.68	J/molxK	969.32	Joback Method
cpg	1129.04	J/molxK	1002.50	Joback Method
cpg	1141.95	J/molxK	1035.69	Joback Method
cpg	1153.41	J/molxK	1068.88	Joback Method
dvisc	0.0006307	Paxs	496.12	Joback Method

dvisc	0.0003197	Paxs	558.39	Joback Method
dvisc	0.0001857	Paxs	620.67	Joback Method
dvisc	0.0001191	Paxs	682.94	Joback Method
dvisc	0.0000823	Paxs	745.21	Joback Method
dvisc	0.0000602	Paxs	807.49	Joback Method
dvisc	0.0000460	Paxs	869.76	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U340032&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U340032&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>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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