

# 1,2-Cyclohexanedicarboxylic acid, allyl heptyl ester

Inchi:	InChI=1S/C18H30O4/c1-3-5-6-7-10-14-22-18(20)16-12-9-8-11-15(16)17(19)21-13-4-2/h4
InchiKey:	SQCHRHSVUHSXTL-UHFFFAOYSA-N
Formula:	C18H30O4
SMILES:	C=CCOC(=O)C1CCCCC1C(=O)OCCCCCCC
Mol. weight [g/mol]:	310.43

## Physical Properties

Property code	Value	Unit	Source
gf	-262.58	kJ/mol	Joback Method
hf	-745.04	kJ/mol	Joback Method
hfus	39.58	kJ/mol	Joback Method
hvap	73.42	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.036		Crippen Method
mvol	264.200	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
tb	775.38	K	Joback Method
tc	971.91	K	Joback Method
tf	438.32	K	Joback Method
vc	1.004	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.59	J/molxK	775.38	Joback Method
cpg	841.18	J/molxK	808.14	Joback Method
cpg	858.55	J/molxK	840.89	Joback Method
cpg	874.73	J/molxK	873.65	Joback Method
cpg	889.73	J/molxK	906.40	Joback Method
cpg	903.57	J/molxK	939.16	Joback Method
cpg	916.25	J/molxK	971.91	Joback Method
dvisc	0.0012385	Paxs	438.32	Joback Method

dvisc	0.0006390	Paxs	494.50	Joback Method
dvisc	0.0003773	Paxs	550.67	Joback Method
dvisc	0.0002457	Paxs	606.85	Joback Method
dvisc	0.0001720	Paxs	663.03	Joback Method
dvisc	0.0001273	Paxs	719.20	Joback Method
dvisc	0.0000984	Paxs	775.38	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U339485&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339485&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>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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