

# Adipic acid, cis-hex-3-enyl isoheptyl ester

<b>Inchi:</b>	InChI=1S/C18H32O4/c1-4-5-6-9-14-21-17(19)12-7-8-13-18(20)22-15-10-11-16(2)3/h5-6,
<b>InchiKey:</b>	MNHKUIFPPUKJDE-WAYWQWQTSA-N
<b>Formula:</b>	C18H32O4
<b>SMILES:</b>	CCC=CCCOC(=O)CCCCC(=O)OCCCC(C)C
<b>Mol. weight [g/mol]:</b>	312.44

## Physical Properties

Property code	Value	Unit	Source
gf	-289.38	kJ/mol	Joback Method
hf	-792.51	kJ/mol	Joback Method
hfus	44.63	kJ/mol	Joback Method
hvap	73.54	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.426		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
rinsol	2106.00		NIST Webbook
tb	767.54	K	Joback Method
tc	951.19	K	Joback Method
tf	416.86	K	Joback Method
vc	1.065	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.70	J/molxK	767.54	Joback Method
cpg	842.72	J/molxK	798.15	Joback Method
cpg	858.83	J/molxK	828.76	Joback Method
cpg	874.04	J/molxK	859.37	Joback Method
cpg	888.37	J/molxK	889.97	Joback Method
cpg	901.84	J/molxK	920.58	Joback Method
cpg	914.48	J/molxK	951.19	Joback Method
dvisc	0.0011565	Paxs	416.86	Joback Method
dvisc	0.0005130	Paxs	475.31	Joback Method

dvisc	0.0002719	Paxs	533.75	Joback Method
dvisc	0.0001633	Paxs	592.20	Joback Method
dvisc	0.0001075	Paxs	650.65	Joback Method
dvisc	0.0000758	Paxs	709.09	Joback Method
dvisc	0.0000564	Paxs	767.54	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U353974&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353974&amp;Units=SI</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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