

# Adipic acid, cis-non-3-enyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C19H34O4/c1-4-5-6-7-8-9-12-15-22-18(20)13-10-11-14-19(21)23-16-17(2)3/h8
<b>InchiKey:</b>	OWGUKJPNAXOSDA-HJWRWDBZSA-N
<b>Formula:</b>	C19H34O4
<b>SMILES:</b>	CCCCC=CCCOC(=O)CCCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	326.47

## Physical Properties

Property code	Value	Unit	Source
gf	-280.96	kJ/mol	Joback Method
hf	-813.15	kJ/mol	Joback Method
hfus	47.22	kJ/mol	Joback Method
hvap	75.77	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.816		Crippen Method
mvol	289.150	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	2183.00		NIST Webbook
rinpol	2183.00		NIST Webbook
tb	790.42	K	Joback Method
tc	975.43	K	Joback Method
tf	428.13	K	Joback Method
vc	1.121	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.58	J/molxK	790.42	Joback Method
cpg	901.98	J/molxK	821.26	Joback Method
cpg	918.41	J/molxK	852.09	Joback Method
cpg	933.89	J/molxK	882.93	Joback Method
cpg	948.47	J/molxK	913.76	Joback Method
cpg	962.14	J/molxK	944.60	Joback Method
cpg	974.95	J/molxK	975.43	Joback Method
dvisc	0.0010369	Paxs	428.13	Joback Method

dvisc	0.0004554	Paxs	488.51	Joback Method
dvisc	0.0002397	Paxs	548.89	Joback Method
dvisc	0.0001433	Paxs	609.27	Joback Method
dvisc	0.0000940	Paxs	669.66	Joback Method
dvisc	0.0000661	Paxs	730.04	Joback Method
dvisc	0.0000490	Paxs	790.42	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=U353990&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353990&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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