

# Adipic acid, butyl pent-4-enyl ester

<b>Inchi:</b>	InChI=1S/C15H26O4/c1-3-5-9-13-19-15(17)11-8-7-10-14(16)18-12-6-4-2/h3H,1,4-13H2,14-18H
<b>InchiKey:</b>	NPCNERQMEQKTQO-UHFFFAOYSA-N
<b>Formula:</b>	C15H26O4
<b>SMILES:</b>	C=CCCCOC(=O)CCCC(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	270.36

## Physical Properties

Property code	Value	Unit	Source
gf	-304.58	kJ/mol	Joback Method
hf	-717.10	kJ/mol	Joback Method
hfus	38.90	kJ/mol	Joback Method
hvap	66.63	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.399		Crippen Method
mvol	232.790	ml/mol	McGowan Method
pc	1569.72	kPa	Joback Method
rinpol	1850.00		NIST Webbook
tb	691.86	K	Joback Method
tc	869.60	K	Joback Method
tf	401.37	K	Joback Method
vc	0.904	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.38	J/molxK	691.86	Joback Method
cpg	668.97	J/molxK	721.48	Joback Method
cpg	683.81	J/molxK	751.11	Joback Method
cpg	697.90	J/molxK	780.73	Joback Method
cpg	711.24	J/molxK	810.35	Joback Method
cpg	723.86	J/molxK	839.98	Joback Method
cpg	735.75	J/molxK	869.60	Joback Method
dvisc	0.0013617	Paxs	401.37	Joback Method
dvisc	0.0007165	Paxs	449.78	Joback Method

dvisc	0.0004271	Paxs	498.20	Joback Method
dvisc	0.0002791	Paxs	546.62	Joback Method
dvisc	0.0001954	Paxs	595.03	Joback Method
dvisc	0.0001444	Paxs	643.44	Joback Method
dvisc	0.0001113	Paxs	691.86	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=U353793&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353793&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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