

# Adipic acid, isobutyl 3-methylbutyl ester

<b>Inchi:</b>	InChI=1S/C15H28O4/c1-12(2)9-10-18-14(16)7-5-6-8-15(17)19-11-13(3)4/h12-13H,5-11H
<b>InchiKey:</b>	GNBNJGYJYNYBK-UHFFFAOYSA-N
<b>Formula:</b>	C15H28O4
<b>SMILES:</b>	CC(C)CCOC(=O)CCCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	272.38

## Physical Properties

Property code	Value	Unit	Source
gf	-397.30	kJ/mol	Joback Method
hf	-853.09	kJ/mol	Joback Method
hfus	33.13	kJ/mol	Joback Method
hvap	66.52	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.335		Crippen Method
mvol	237.090	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook
tb	694.30	K	Joback Method
tc	874.56	K	Joback Method
tf	373.13	K	Joback Method
vc	0.911	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.23	J/molxK	694.30	Joback Method
cpg	752.95	J/molxK	844.52	Joback Method
cpg	739.62	J/molxK	814.47	Joback Method
cpg	725.49	J/molxK	784.43	Joback Method
cpg	710.56	J/molxK	754.39	Joback Method
cpg	694.81	J/molxK	724.34	Joback Method
cpg	765.47	J/molxK	874.56	Joback Method
dvisc	0.0000905	Paxs	694.30	Joback Method

dvisc	0.0001227	Paxs	640.77	Joback Method
dvisc	0.0001760	Paxs	587.24	Joback Method
dvisc	0.0002714	Paxs	533.71	Joback Method
dvisc	0.0004608	Paxs	480.19	Joback Method
dvisc	0.0008937	Paxs	426.66	Joback Method
dvisc	0.0020958	Paxs	373.13	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=U348455&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348455&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>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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