

# Adipic acid, 3,3-dimethylbut-2-yl heptyl ester

<b>Inchi:</b>	InChI=1S/C19H36O4/c1-6-7-8-9-12-15-22-17(20)13-10-11-14-18(21)23-16(2)19(3,4)5/h1
<b>InchiKey:</b>	BAFMJYQCAHVRL-UHFFFAOYSA-N
<b>Formula:</b>	C19H36O4
<b>SMILES:</b>	CCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	328.49

## Physical Properties

Property code	Value	Unit	Source
gf	-358.34	kJ/mol	Joback Method
hf	-939.12	kJ/mol	Joback Method
hfus	39.60	kJ/mol	Joback Method
hvap	74.52	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	5.038		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinsol	2106.00		NIST Webbook
tb	783.03	K	Joback Method
tc	968.31	K	Joback Method
tf	435.63	K	Joback Method
vc	1.131	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.66	J/molxK	783.03	Joback Method
cpg	928.69	J/molxK	813.91	Joback Method
cpg	945.69	J/molxK	844.79	Joback Method
cpg	961.70	J/molxK	875.67	Joback Method
cpg	976.73	J/molxK	906.55	Joback Method
cpg	990.82	J/molxK	937.43	Joback Method
cpg	1004.00	J/molxK	968.31	Joback Method
dvisc	0.0010903	Paxs	435.63	Joback Method
dvisc	0.0004713	Paxs	493.53	Joback Method

dvisc	0.0002430	Paxs	551.43	Joback Method
dvisc	0.0001421	Paxs	609.33	Joback Method
dvisc	0.0000912	Paxs	667.23	Joback Method
dvisc	0.0000628	Paxs	725.13	Joback Method
dvisc	0.0000457	Paxs	783.03	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=U353672&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353672&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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