

# Adipic acid, 3-methylbut-3-enyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C24H44O4/c1-4-5-6-7-8-9-10-11-12-13-16-20-27-23(25)17-14-15-18-24(26)28
<b>InchiKey:</b>	LBSCAKPFLCPMFB-UHFFFAOYSA-N
<b>Formula:</b>	C24H44O4
<b>SMILES:</b>	<chem>C=C(C)CCOC(=O)CCCC(=O)OCCCCCCCCCCCCC</chem>
<b>Mol. weight [g/mol]:</b>	396.60

## Physical Properties

Property code	Value	Unit	Source
gf	-237.35	kJ/mol	Joback Method
hf	-912.65	kJ/mol	Joback Method
hfus	60.90	kJ/mol	Joback Method
hvap	86.74	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.910		Crippen Method
mcvol	359.600	ml/mol	McGowan Method
pc	873.77	kPa	Joback Method
rinqol	2716.00		NIST Webbook
tb	897.66	K	Joback Method
tc	1099.45	K	Joback Method
tf	488.84	K	Joback Method
vc	1.409	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.31	J/mol×K	897.66	Joback Method
cpg	1207.87	J/mol×K	931.29	Joback Method
cpg	1226.11	J/mol×K	964.92	Joback Method
cpg	1243.07	J/mol×K	998.55	Joback Method
cpg	1258.78	J/mol×K	1032.19	Joback Method
cpg	1273.28	J/mol×K	1065.82	Joback Method
cpg	1286.62	J/mol×K	1099.45	Joback Method

# Sources

<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=U354036&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354036&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rinpola:</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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