

# Adipic acid, «beta»-citronellyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C29H54O4/c1-5-6-7-8-9-10-11-12-13-14-17-24-32-28(30)21-15-16-22-29(31)3
<b>InchiKey:</b>	URSBKNYPEDFOPV-UHFFFAOYSA-N
<b>Formula:</b>	C29H54O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCCC(=O)OCCC(C)CCC=C(C)C
<b>Mol. weight [g/mol]:</b>	466.74

## Physical Properties

Property code	Value	Unit	Source
gf	-205.31	kJ/mol	Joback Method
hf	-1029.34	kJ/mol	Joback Method
hfus	71.81	kJ/mol	Joback Method
hvap	98.11	kJ/mol	Joback Method
log10ws	-9.30		Crippen Method
logp	8.717		Crippen Method
mvol	430.050	ml/mol	McGowan Method
pc	676.41	kPa	Joback Method
rinpol	3166.00		NIST Webbook
rinpol	3166.00		NIST Webbook
tb	1019.10	K	Joback Method
tc	1263.92	K	Joback Method
tf	526.87	K	Joback Method
vc	1.683	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1511.42	J/molxK	1019.10	Joback Method
cpg	1533.94	J/molxK	1059.90	Joback Method
cpg	1554.56	J/molxK	1100.71	Joback Method
cpg	1573.37	J/molxK	1141.51	Joback Method
cpg	1590.49	J/molxK	1182.31	Joback Method
cpg	1606.00	J/molxK	1223.12	Joback Method
cpg	1620.02	J/molxK	1263.92	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=U353776&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353776&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>h vap:</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>r in pol:</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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