

# Adipic acid, «beta»-citronellyl pentadecyl ester

Inchi:	InChI=1S/C31H58O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-19-26-34-30(32)23-17-18-24-3
InchiKey:	UWHNXSUQQGGPQW-UHFFFAOYSA-N
Formula:	C31H58O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]:	494.79

## Physical Properties

Property code	Value	Unit	Source
gf	-188.47	kJ/mol	Joback Method
hf	-1070.62	kJ/mol	Joback Method
hfus	76.99	kJ/mol	Joback Method
hvap	102.56	kJ/mol	Joback Method
log10ws	-10.14		Crippen Method
logp	9.497		Crippen Method
mvol	458.230	ml/mol	McGowan Method
pc	613.60	kPa	Joback Method
rinpol	3367.00		NIST Webbook
rinpol	3367.00		NIST Webbook
tb	1064.86	K	Joback Method
tc	1335.88	K	Joback Method
tf	549.41	K	Joback Method
vc	1.794	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1642.42	J/mol×K	1064.86	Joback Method
cpg	1666.59	J/mol×K	1110.03	Joback Method
cpg	1688.47	J/mol×K	1155.20	Joback Method
cpg	1708.19	J/mol×K	1200.37	Joback Method
cpg	1725.92	J/mol×K	1245.54	Joback Method
cpg	1741.81	J/mol×K	1290.71	Joback Method
cpg	1756.01	J/mol×K	1335.88	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=U353778&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353778&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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