

# Adipic acid, «beta»-citronellyl tetradecyl ester

<b>Inchi:</b>	InChI=1S/C30H56O4/c1-5-6-7-8-9-10-11-12-13-14-15-18-25-33-29(31)22-16-17-23-30(3
<b>InchiKey:</b>	PLHZYVHXJZJSTE-UHFFFAOYSA-N
<b>Formula:</b>	C30H56O4
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)CCCC(=O)OCCC(C)CCC=C(C)C
<b>Mol. weight [g/mol]:</b>	480.76

## Physical Properties

Property code	Value	Unit	Source
gf	-196.89	kJ/mol	Joback Method
hf	-1049.98	kJ/mol	Joback Method
hfus	74.40	kJ/mol	Joback Method
hvap	100.34	kJ/mol	Joback Method
log10ws	-9.72		Crippen Method
logp	9.107		Crippen Method
mcvol	444.140	ml/mol	McGowan Method
pc	643.85	kPa	Joback Method
rinsol	3267.00		NIST Webbook
tb	1041.98	K	Joback Method
tc	1299.12	K	Joback Method
tf	538.14	K	Joback Method
vc	1.738	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1576.77	J/mol×K	1041.98	Joback Method
cpg	1600.08	J/mol×K	1084.84	Joback Method
cpg	1621.31	J/mol×K	1127.69	Joback Method
cpg	1640.56	J/mol×K	1170.55	Joback Method
cpg	1657.97	J/mol×K	1213.40	Joback Method
cpg	1673.67	J/mol×K	1256.26	Joback Method
cpg	1687.78	J/mol×K	1299.12	Joback Method

# Sources

<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=U353777&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353777&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>
<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>

# 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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