

# Adipic acid, «beta»-citronellyl decyl ester

<b>Inchi:</b>	InChI=1S/C26H48O4/c1-5-6-7-8-9-10-11-14-21-29-25(27)18-12-13-19-26(28)30-22-20-2
<b>InchiKey:</b>	RDJBMEASUYNYQI-UHFFFAOYSA-N
<b>Formula:</b>	C26H48O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCC(=O)OCCC(C)CCC=C(C)C
<b>Mol. weight [g/mol]:</b>	424.66

## Physical Properties

Property code	Value	Unit	Source
gf	-230.57	kJ/mol	Joback Method
hf	-967.42	kJ/mol	Joback Method
hfus	64.04	kJ/mol	Joback Method
hvap	91.43	kJ/mol	Joback Method
log10ws	-8.04		Crippen Method
logp	7.546		Crippen Method
mvol	387.780	ml/mol	McGowan Method
pc	790.37	kPa	Joback Method
rinpol	2861.00		NIST Webbook
tb	950.46	K	Joback Method
tc	1166.63	K	Joback Method
tf	493.06	K	Joback Method
vc	1.514	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1317.56	J/mol×K	950.46	Joback Method
cpg	1338.10	J/mol×K	986.49	Joback Method
cpg	1357.16	J/mol×K	1022.52	Joback Method
cpg	1374.79	J/mol×K	1058.54	Joback Method
cpg	1391.06	J/mol×K	1094.57	Joback Method
cpg	1406.04	J/mol×K	1130.60	Joback Method
cpg	1419.77	J/mol×K	1166.63	Joback Method

# Sources

<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>
<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=U353773&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353773&amp;Units=SI</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>mccvol:</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

Latest version available from:

<https://www.chemeo.com/cid/31-480-4/Adipic-acid-beta-citronellyl-decyl-ester.pdf>

Generated by Cheméo on 2024-04-27 10:54:28.746937279 +0000 UTC m=+16504517.667514594.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.