

# Adipic acid, decyl 3-ethylphenyl ester

<b>Inchi:</b>	InChI=1S/C24H38O4/c1-3-5-6-7-8-9-10-13-19-27-23(25)17-11-12-18-24(26)28-22-16-14
<b>InchiKey:</b>	XYIVUTMJUAVQNE-UHFFFAOYSA-N
<b>Formula:</b>	C24H38O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCC(=O)Oc1cccc(CC)c1
<b>Mol. weight [g/mol]:</b>	390.56

## Physical Properties

Property code	Value	Unit	Source
gf	-213.86	kJ/mol	Joback Method
hf	-803.23	kJ/mol	Joback Method
hfus	57.14	kJ/mol	Joback Method
hvap	90.27	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	6.399		Crippen Method
mvol	340.140	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	2845.00		NIST Webbook
rinpol	2845.00		NIST Webbook
tb	932.76	K	Joback Method
tc	1142.45	K	Joback Method
tf	543.50	K	Joback Method
vc	1.319	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.44	J/molxK	932.76	Joback Method
cpg	1136.46	J/molxK	967.71	Joback Method
cpg	1152.13	J/molxK	1002.66	Joback Method
cpg	1166.46	J/molxK	1037.60	Joback Method
cpg	1179.51	J/molxK	1072.55	Joback Method
cpg	1191.30	J/molxK	1107.50	Joback Method
cpg	1201.88	J/molxK	1142.45	Joback Method
dvisc	0.0003848	Paxs	543.50	Joback Method

dvisc	0.0002018	Paxs	608.38	Joback Method
dvisc	0.0001199	Paxs	673.25	Joback Method
dvisc	0.0000780	Paxs	738.13	Joback Method
dvisc	0.0000544	Paxs	803.01	Joback Method
dvisc	0.0000401	Paxs	867.88	Joback Method
dvisc	0.0000308	Paxs	932.76	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=U353900&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353900&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mcvol:</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

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