

# Adipic acid, 2-chloro-5-methylphenyl undecyl ester

Inchi:	InChI=1S/C24H37ClO4/c1-3-4-5-6-7-8-9-10-13-18-28-23(26)14-11-12-15-24(27)29-22-19
InchiKey:	RUBBYTOEECFHMJ-UHFFFAOYSA-N
Formula:	C24H37ClO4
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	425.00

## Physical Properties

Property code	Value	Unit	Source
gf	-235.42	kJ/mol	Joback Method
hf	-830.44	kJ/mol	Joback Method
hfus	60.95	kJ/mol	Joback Method
hvap	95.32	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.188		Crippen Method
mvol	352.380	ml/mol	McGowan Method
pc	997.65	kPa	Joback Method
rinpol	3046.00		NIST Webbook
rinpol	3046.00		NIST Webbook
tb	975.17	K	Joback Method
tc	1193.89	K	Joback Method
tf	585.94	K	Joback Method
vc	1.369	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1145.33	J/molxK	975.17	Joback Method
cpg	1161.08	J/molxK	1011.62	Joback Method
cpg	1175.39	J/molxK	1048.08	Joback Method
cpg	1188.30	J/molxK	1084.53	Joback Method
cpg	1199.85	J/molxK	1120.98	Joback Method
cpg	1210.07	J/molxK	1157.44	Joback Method
cpg	1219.02	J/molxK	1193.89	Joback Method
dvisc	0.0002714	Paxs	585.94	Joback Method

dvisc	0.0001520	Paxs	650.81	Joback Method
dvisc	0.0000945	Paxs	715.68	Joback Method
dvisc	0.0000636	Paxs	780.56	Joback Method
dvisc	0.0000455	Paxs	845.43	Joback Method
dvisc	0.0000341	Paxs	910.30	Joback Method
dvisc	0.0000266	Paxs	975.17	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U353966&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353966&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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