

# Adipic acid, decyl trans-hex-3-enyl ester

<b>Inchi:</b>	InChI=1S/C22H40O4/c1-3-5-7-9-10-11-12-16-20-26-22(24)18-14-13-17-21(23)25-19-15-
<b>InchiKey:</b>	PMATXCIZZIHHSO-SOFGYWHQSA-N
<b>Formula:</b>	C22H40O4
<b>SMILES:</b>	CCC=CCCOC(=O)CCCCC(=O)OCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	368.55

## Physical Properties

Property code	Value	Unit	Source
gf	-253.26	kJ/mol	Joback Method
hf	-869.79	kJ/mol	Joback Method
hfus	58.51	kJ/mol	Joback Method
hvap	82.84	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.130		Crippen Method
mvol	331.420	ml/mol	McGowan Method
pc	985.16	kPa	Joback Method
rinpol	2526.00		NIST Webbook
rinpol	2526.00		NIST Webbook
tb	859.50	K	Joback Method
tc	1052.62	K	Joback Method
tf	476.94	K	Joback Method
vc	1.296	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.82	J/molxK	859.50	Joback Method
cpg	1084.38	J/molxK	891.69	Joback Method
cpg	1101.82	J/molxK	923.87	Joback Method
cpg	1118.16	J/molxK	956.06	Joback Method
cpg	1133.46	J/molxK	988.25	Joback Method
cpg	1147.73	J/molxK	1020.43	Joback Method
cpg	1161.02	J/molxK	1052.62	Joback Method
dvisc	0.0006226	Paxs	476.94	Joback Method

dvisc	0.0002897	Paxs	540.70	Joback Method
dvisc	0.0001584	Paxs	604.46	Joback Method
dvisc	0.0000972	Paxs	668.22	Joback Method
dvisc	0.0000649	Paxs	731.98	Joback Method
dvisc	0.0000463	Paxs	795.74	Joback Method
dvisc	0.0000347	Paxs	859.50	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U354014&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354014&amp;Units=SI</a>

## Legend

<b>cpg:</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>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>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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