

# Fumaric acid, 3-hexyl undecyl ester

<b>Inchi:</b>	InChI=1S/C21H38O4/c1-4-7-8-9-10-11-12-13-14-18-24-20(22)16-17-21(23)25-19(6-3)15
<b>InchiKey:</b>	JZGMPIWQICJSKS-WUKNDPDISA-N
<b>Formula:</b>	C21H38O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C=CC(=O)OC(CC)CCC
<b>Mol. weight [g/mol]:</b>	354.52

## Physical Properties

Property code	Value	Unit	Source
gf	-264.12	kJ/mol	Joback Method
hf	-854.43	kJ/mol	Joback Method
hfus	52.40	kJ/mol	Joback Method
hvap	80.22	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.739		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
tb	836.18	K	Joback Method
tc	1026.01	K	Joback Method
tf	450.67	K	Joback Method
vc	1.234	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.95	J/molxK	836.18	Joback Method
cpg	1023.11	J/molxK	867.82	Joback Method
cpg	1040.19	J/molxK	899.46	Joback Method
cpg	1056.24	J/molxK	931.09	Joback Method
cpg	1071.28	J/molxK	962.73	Joback Method
cpg	1085.33	J/molxK	994.37	Joback Method
cpg	1098.44	J/molxK	1026.01	Joback Method
dvisc	0.0008233	Paxs	450.67	Joback Method

dvisc	0.0003550	Paxs	514.92	Joback Method
dvisc	0.0001845	Paxs	579.17	Joback Method
dvisc	0.0001092	Paxs	643.42	Joback Method
dvisc	0.0000712	Paxs	707.68	Joback Method
dvisc	0.0000498	Paxs	771.93	Joback Method
dvisc	0.0000368	Paxs	836.18	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U348610&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348610&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>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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