

# Fumaric acid, cis-hex-3-enyl heptadecyl ester

**Inchi:** InChI=1S/C27H48O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-21-25-31-27(29)23-22-  
**InchiKey:** WUNDBFSYURGPIV-FXWCUKDTSA-N  
**Formula:** C27H48O4  
**SMILES:** CCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCCCCC  
**Mol. weight [g/mol]:** 436.67

## Physical Properties

Property code	Value	Unit	Source
gf	-130.94	kJ/mol	Joback Method
hf	-855.77	kJ/mol	Joback Method
hfus	71.66	kJ/mol	Joback Method
hvap	93.92	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	7.857		Crippen Method
mcvol	397.570	ml/mol	McGowan Method
pc	765.64	kPa	Joback Method
rinpol	3094.00		NIST Webbook
tb	978.06	K	Joback Method
tc	1203.84	K	Joback Method
tf	528.21	K	Joback Method
vc	1.556	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1353.80	J/molxK	978.06	Joback Method
cpg	1374.69	J/molxK	1015.69	Joback Method
cpg	1394.13	J/molxK	1053.32	Joback Method
cpg	1412.23	J/molxK	1090.95	Joback Method
cpg	1429.06	J/molxK	1128.58	Joback Method
cpg	1444.72	J/molxK	1166.21	Joback Method
cpg	1459.30	J/molxK	1203.84	Joback Method
dvisc	0.0003108	Paxs	528.21	Joback Method
dvisc	0.0001350	Paxs	603.19	Joback Method

dvisc	0.0000706	Paxs	678.16	Joback Method
dvisc	0.0000419	Paxs	753.13	Joback Method
dvisc	0.0000274	Paxs	828.11	Joback Method
dvisc	0.0000192	Paxs	903.09	Joback Method
dvisc	0.0000142	Paxs	978.06	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U348872&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348872&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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