

# Fumaric acid, heptadecyl 3-hexyl ester

<b>Inchi:</b>	InChI=1S/C27H50O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-30-26(28)22-23-
<b>InchiKey:</b>	OZMLZUDUAQCTTE-GHVJWSGMSA-N
<b>Formula:</b>	C27H50O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)CCC
<b>Mol. weight [g/mol]:</b>	438.68

## Physical Properties

Property code	Value	Unit	Source
gf	-213.60	kJ/mol	Joback Method
hf	-978.27	kJ/mol	Joback Method
hfus	67.94	kJ/mol	Joback Method
hvap	93.58	kJ/mol	Joback Method
log10ws	-8.82		Crippen Method
logp	8.079		Crippen Method
mvol	401.870	ml/mol	McGowan Method
pc	747.33	kPa	Joback Method
rinpol	2990.00		NIST Webbook
tb	973.46	K	Joback Method
tc	1199.13	K	Joback Method
tf	518.29	K	Joback Method
vc	1.569	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1382.13	J/molxK	973.46	Joback Method
cpg	1403.35	J/molxK	1011.07	Joback Method
cpg	1422.94	J/molxK	1048.68	Joback Method
cpg	1440.98	J/molxK	1086.29	Joback Method
cpg	1457.52	J/molxK	1123.90	Joback Method
cpg	1472.65	J/molxK	1161.52	Joback Method
cpg	1486.45	J/molxK	1199.13	Joback Method
dvisc	0.0003810	Paxs	518.29	Joback Method
dvisc	0.0001568	Paxs	594.15	Joback Method

dvisc	0.0000789	Paxs	670.01	Joback Method
dvisc	0.0000457	Paxs	745.88	Joback Method
dvisc	0.0000292	Paxs	821.74	Joback Method
dvisc	0.0000202	Paxs	897.60	Joback Method
dvisc	0.0000148	Paxs	973.46	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=U348615&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348615&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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