

# Fumaric acid, 3-heptyl nonadecyl ester

<b>Inchi:</b>	InChI=1S/C30H56O4/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-27-33-29(31
<b>InchiKey:</b>	PAZHSWNZBVLHL-OCEACIFDSA-N
<b>Formula:</b>	C30H56O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)CCCC
<b>Mol. weight [g/mol]:</b>	480.76

## Physical Properties

Property code	Value	Unit	Source
gf	-188.34	kJ/mol	Joback Method
hf	-1040.19	kJ/mol	Joback Method
hfus	75.71	kJ/mol	Joback Method
hvap	100.26	kJ/mol	Joback Method
log10ws	-10.07		Crippen Method
logp	9.249		Crippen Method
mvol	444.140	ml/mol	McGowan Method
pc	642.22	kPa	Joback Method
rinpol	3273.00		NIST Webbook
rinpol	3273.00		NIST Webbook
tb	1042.10	K	Joback Method
tc	1301.69	K	Joback Method
tf	552.10	K	Joback Method
vc	1.738	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1577.07	J/molxK	1042.10	Joback Method
cpg	1600.54	J/molxK	1085.36	Joback Method
cpg	1621.87	J/molxK	1128.63	Joback Method
cpg	1641.18	J/molxK	1171.89	Joback Method
cpg	1658.60	J/molxK	1215.16	Joback Method
cpg	1674.27	J/molxK	1258.42	Joback Method
cpg	1688.31	J/molxK	1301.69	Joback Method
dvisc	0.0002504	Paxs	552.10	Joback Method

dvisc	0.0001011	Paxs	633.77	Joback Method
dvisc	0.0000502	Paxs	715.43	Joback Method
dvisc	0.0000288	Paxs	797.10	Joback Method
dvisc	0.0000183	Paxs	878.77	Joback Method
dvisc	0.0000126	Paxs	960.43	Joback Method
dvisc	0.0000092	Paxs	1042.10	Joback Method

## Sources

<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=U348696&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348696&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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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

Latest version available from:

<https://www.chemeo.com/cid/37-713-9/Fumaric-acid-3-heptyl-nonadecyl-ester.pdf>

Generated by Cheméo on 2024-04-24 04:23:52.837681654 +0000 UTC m=+16221881.758258982.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.