

# Fumaric acid, dec-4-enyl propyl ester

<b>Inchi:</b>	InChI=1S/C17H28O4/c1-3-5-6-7-8-9-10-11-15-21-17(19)13-12-16(18)20-14-4-2/h8-9,12-
<b>InchiKey:</b>	KRWQCOUOOVIGML-AFAJWACHSA-N
<b>Formula:</b>	C17H28O4
<b>SMILES:</b>	CCCCC=CCCCOC(=O)C=CC(=O)OCCC
<b>Mol. weight [g/mol]:</b>	296.40

## Physical Properties

Property code	Value	Unit	Source
gf	-215.14	kJ/mol	Joback Method
hf	-649.37	kJ/mol	Joback Method
hfus	45.76	kJ/mol	Joback Method
hvap	71.66	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.956		Crippen Method
mvol	256.670	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
tb	749.26	K	Joback Method
tc	934.62	K	Joback Method
tf	415.51	K	Joback Method
vc	0.996	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.30	J/molxK	749.26	Joback Method
cpg	814.98	J/molxK	903.72	Joback Method
cpg	802.20	J/molxK	872.83	Joback Method
cpg	788.68	J/molxK	841.94	Joback Method
cpg	774.37	J/molxK	811.05	Joback Method
cpg	759.26	J/molxK	780.15	Joback Method
cpg	827.02	J/molxK	934.62	Joback Method
dvisc	0.0000607	Paxs	749.26	Joback Method

dvisc	0.0000802	Paxs	693.63	Joback Method
dvisc	0.0001112	Paxs	638.01	Joback Method
dvisc	0.0001642	Paxs	582.38	Joback Method
dvisc	0.0002631	Paxs	526.76	Joback Method
dvisc	0.0004712	Paxs	471.14	Joback Method
dvisc	0.0009864	Paxs	415.51	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U348936&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348936&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>mccvol:</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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