

# Fumaric acid, nonyl 3-oxobut-2-yl ester

<b>Inchi:</b>	InChI=1S/C17H28O5/c1-4-5-6-7-8-9-10-13-21-16(19)11-12-17(20)22-15(3)14(2)18/h11-16
<b>InchiKey:</b>	DGZGWSFAYNREFH-VAWYXSNFSA-N
<b>Formula:</b>	C17H28O5
<b>SMILES:</b>	CCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
<b>Mol. weight [g/mol]:</b>	312.40

## Physical Properties

Property code	Value	Unit	Source
gf	-426.72	kJ/mol	Joback Method
hf	-884.45	kJ/mol	Joback Method
hfus	43.64	kJ/mol	Joback Method
hvap	78.06	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.357		Crippen Method
mvol	262.540	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		NIST Webbook
tb	798.53	K	Joback Method
tc	989.55	K	Joback Method
tf	455.52	K	Joback Method
vc	1.016	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.93	J/molxK	798.53	Joback Method
cpg	804.20	J/molxK	830.37	Joback Method
cpg	818.54	J/molxK	862.20	Joback Method
cpg	831.97	J/molxK	894.04	Joback Method
cpg	844.51	J/molxK	925.87	Joback Method
cpg	856.19	J/molxK	957.71	Joback Method
cpg	867.02	J/molxK	989.55	Joback Method
dvisc	0.0009665	Paxs	455.52	Joback Method

dvisc	0.0004743	Paxs	512.69	Joback Method
dvisc	0.0002685	Paxs	569.86	Joback Method
dvisc	0.0001686	Paxs	627.02	Joback Method
dvisc	0.0001144	Paxs	684.19	Joback Method
dvisc	0.0000825	Paxs	741.36	Joback Method
dvisc	0.0000623	Paxs	798.53	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=U348823&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348823&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>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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