

# Fumaric acid, ethyl 1-phenylprop-1-yl ester

<b>Inchi:</b>	InChI=1S/C15H18O4/c1-3-13(12-8-6-5-7-9-12)19-15(17)11-10-14(16)18-4-2/h5-11,13H,3
<b>InchiKey:</b>	XDHCCSALIVGTBU-ZHACJKMWSA-N
<b>Formula:</b>	C15H18O4
<b>SMILES:</b>	CCOC(=O)C=CC(=O)OC(CC)c1ccccc1
<b>Mol. weight [g/mol]:</b>	262.30

## Physical Properties

Property code	Value	Unit	Source
gf	-202.23	kJ/mol	Joback Method
hf	-494.06	kJ/mol	Joback Method
hfus	30.90	kJ/mol	Joback Method
hvap	69.14	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.800		Crippen Method
mcvol	209.030	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinqol	1853.00		NIST Webbook
tb	725.58	K	Joback Method
tc	938.71	K	Joback Method
tf	409.47	K	Joback Method
vc	0.789	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.20	J/molxK	725.58	Joback Method
cpg	634.58	J/molxK	903.18	Joback Method
cpg	623.78	J/molxK	867.66	Joback Method
cpg	612.07	J/molxK	832.14	Joback Method
cpg	599.42	J/molxK	796.62	Joback Method
cpg	585.81	J/molxK	761.10	Joback Method
cpg	644.51	J/molxK	938.71	Joback Method
dvisc	0.0000844	Paxs	725.58	Joback Method
dvisc	0.0001106	Paxs	672.89	Joback Method

dvisc	0.0001517	Paxs	620.21	Joback Method
dvisc	0.0002208	Paxs	567.52	Joback Method
dvisc	0.0003470	Paxs	514.84	Joback Method
dvisc	0.0006045	Paxs	462.16	Joback Method
dvisc	0.0012147	Paxs	409.47	Joback Method

## Sources

<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=U405908&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405908&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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