

# Fumaric acid, ethyl 4-methylpent-2-yl ester

<b>Inchi:</b>	InChI=1S/C12H20O4/c1-5-15-11(13)6-7-12(14)16-10(4)8-9(2)3/h6-7,9-10H,5,8H2,1-4H3
<b>InchiKey:</b>	JAZFCTLILMMPGA-VOTSOKGWSA-N
<b>Formula:</b>	C12H20O4
<b>SMILES:</b>	CCOC(=O)C=CC(=O)OC(C)CC(C)C
<b>Mol. weight [g/mol]:</b>	228.28

## Physical Properties

Property code	Value	Unit	Source
gf	-342.34	kJ/mol	Joback Method
hf	-673.95	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hvap	59.80	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.083		Crippen Method
mvol	190.520	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
tb	629.82	K	Joback Method
tc	819.69	K	Joback Method
tf	334.24	K	Joback Method
vc	0.724	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.92	J/molxK	629.82	Joback Method
cpg	510.56	J/molxK	661.47	Joback Method
cpg	524.47	J/molxK	693.11	Joback Method
cpg	537.67	J/molxK	724.76	Joback Method
cpg	550.18	J/molxK	756.40	Joback Method
cpg	561.99	J/molxK	788.05	Joback Method
cpg	573.11	J/molxK	819.69	Joback Method
dvisc	0.0025822	Paxs	334.24	Joback Method

dvisc	0.0010964	Paxs	383.50	Joback Method
dvisc	0.0005658	Paxs	432.77	Joback Method
dvisc	0.0003343	Paxs	482.03	Joback Method
dvisc	0.0002177	Paxs	531.29	Joback Method
dvisc	0.0001525	Paxs	580.56	Joback Method
dvisc	0.0001129	Paxs	629.82	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=U348316&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348316&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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