

# Fumaric acid, ethyl 2-propylphenyl ester

<b>Inchi:</b>	InChI=1S/C15H18O4/c1-3-7-12-8-5-6-9-13(12)19-15(17)11-10-14(16)18-4-2/h5-6,8-11H,
<b>InchiKey:</b>	DMSJLMOZKHOUHPH-ZHACJKMWSA-N
<b>Formula:</b>	C15H18O4
<b>SMILES:</b>	CCCc1ccccc1OC(=O)C=CC(=O)OCC
<b>Mol. weight [g/mol]:</b>	262.30

## Physical Properties

Property code	Value	Unit	Source
gf	-209.42	kJ/mol	Joback Method
hf	-500.25	kJ/mol	Joback Method
hfus	34.03	kJ/mol	Joback Method
hvap	70.19	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.664		Crippen Method
mcvol	209.030	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinqol	1872.00		NIST Webbook
tb	731.00	K	Joback Method
tc	941.42	K	Joback Method
tf	436.99	K	Joback Method
vc	0.795	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.67	J/molxK	731.00	Joback Method
cpg	583.91	J/molxK	766.07	Joback Method
cpg	597.21	J/molxK	801.14	Joback Method
cpg	609.60	J/molxK	836.21	Joback Method
cpg	621.10	J/molxK	871.28	Joback Method
cpg	631.74	J/molxK	906.35	Joback Method
cpg	641.54	J/molxK	941.42	Joback Method
dvisc	0.0008463	Paxs	436.99	Joback Method
dvisc	0.0004844	Paxs	485.99	Joback Method

dvisc	0.0003071	Paxs	534.99	Joback Method
dvisc	0.0002102	Paxs	584.00	Joback Method
dvisc	0.0001526	Paxs	633.00	Joback Method
dvisc	0.0001160	Paxs	682.00	Joback Method
dvisc	0.0000914	Paxs	731.00	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U348123&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348123&amp;Units=SI</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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